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Analytical models of austenite transformation in steels taking into account internal stresses

Abstract

Analytical models of the transformation of austenite into steel are considered, taking into account the influence of the stress state on structural transitions during heat treatment of steels. A simple theoretical expression is proposed for calculating the amount of martensite, formed as a function of the stresses in the γ- phase

Keywords: austenite transformations, analytical models, internal stresses, degree of conversion phases, steels

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Abbreviations: TTT, thermokinetic diagrams; CCT, consists in building isothermal

Introduction

Experimental study of structural transformations of steel as a result of heat treatment consists in building isothermal (CCT) and thermokinetic diagrams (TTT), as well as studying its hardenability.[1,2] At the same time, experimental study of structural transformations has limited application. CCT diagrams are used only to qualitatively assess the influence of the chemical composition on the process of austenite decomposition. TTT diagrams cannot provide reliable information about the structure of steel, if the cooling mode differs from the cooling modes in experiments. For this reason, TTT diagrams are used only to quantify the stability of austenite with continuous cooling. In the field of modeling the kinetics of phase transformations, the most fundamental studies were carried out in the works of A.N. Kolmogorov and M. Avrami, who describe analytical equations, where the volume of the newly formed phase is made dependent on the probability of nucleation of centers, the linear velocity of their growth and the elapsed time.[3,4] Fundamental reviews of mathematical modeling of the phase transformation process are presented in[1,5,6] in which it is indicated that the existing analytical models do not explicitly take into account the process of non-stationary nucleation, and this contradicts the physics of the process. It is also noted that analytical models do not allow to consider the process of formation of individual grains and their growth. In addition to analytical models, there is an approach consisting in imitating the process of nucleation and growth based on the model of I.L. Mirkin, in which it is proposed to study the crystallization process using two-dimensional schemes.[7] The model takes into account the stochastic nature of the process, the incubation period and allows you to get the grain size. At the same time, the stochastic nature of the formation of crystallization centers in the model is not fully implemented. In this model, the space of the melt and crystals is represented as a set of elementary fragments, like a raster image in computer graphics, which makes it difficult to implement the model in three-dimensional space, as well as describing the process in continuous space and time.

In[8–10] the authors developed a diffusion model for the transformation of austenite, based on the use of the physical principles of thermodynamics. The obtained equations for the rate of perlite formation and the inter-plate distance from the supercooling value with a high degree correspond to the experimental data for carbon steels. In[11] a procedure was proposed for calculating structural transformations with arbitrary cooling by CCT diagrams, in which an additivity rule is used to go from isothermal transformation kinetics to non-stationary temperature conditions. This rule is valid for isokinetic reactions, i.e., those for which the process speed depends only on V and t, and not on the "thermal trajectory" along which the system came to this state. In this case, the isothermal kinetics of the processes of nucleation and growth is usually described by the Avrami equation:[9]

$$V_{\alpha} = 1 - exp\left(-K\tau^{n}\right) \qquad (1)$$

where K, n - coefficients, depending on the type of CCT diagrams; V_{α} is the volume fraction of the product of transformation.The Avrami equation, or, as it is also called, Kolmogorov-Johnson-Meil-Avrami[6,7] is used in many mathematical models describing the transformation of austenite (see, for example).[11–14] The additivity of the reaction is as follows: if at the temperature t_1, during τ_1, the volume fraction of the decay product is $V = f(t_1, \tau_1)$, and then the temperature changes abruptly to t_2, then the course of transformation will be described by kinetics:

$$V = f(t_2, t + \tau_2 - \tau_1) \qquad (2)$$

where τ_2 is the time required to achieve the degree of conversion of V_1 at t_2.The described method was used in[15] which equation (1) was applied to describe the decay of austenite in both the pearlitic and bainite regions. The calculation results for the pearlite transformation are consistent with experimental data. However, the interval of the bainite transformation, determined experimentally, is higher than it is predicted by using the additivity rule. This correlates with the

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results of,[16–18] confirming that the processes occurring in supercooled austenite during the incubation period of the pearlite transformation in its upper region, cause an acceleration of the subsequent bainite transformation. To account for this effect, it was proposed to shift the bainitic area on CCT diagrams to the left, depending on the cooling history, according to the formulas

$$\tau^{j}{}_{\text{í B}} = \tau^{1-aJ}{}_{\text{í B}}, \tau^{j}{}_{\text{í B}} / \tau^{j}{}_{\hat{\text{e}}\text{B}} = \tau_{\text{í B}} / \tau_{\hat{\text{e}}\text{B}} \qquad (3)$$

where τ_{nB} and τ^{j}_{nB} is the time of the beginning (end) of the bainite transformation with instant cooling to the holding temperature and with continuous cooling, respectively; a is a parameter depending on the chemical composition of the steel; j is a dimensionless quantity. With the help of a numerical experiment, the values of the parameter a for some steel grades were determined from the condition for better agreement of the experimental and calculated data. The analysis of the presented works shows that mathematical modeling of austenite decomposition during heat treatment is possible using both TTT diagrams and CCT diagrams. In the first case, the use of kinetic models is preferable. In the second, it is advisable to apply the theory of isokinetic reactions. A common drawback of the works described above is the neglect of the effect of the stress-strain state arising during the heat treatment of parts on the kinetics of structural transformations, while the available experimental data[19–22] indicate a significant effect of stresses and strains on structural transformations. The purpose of this paper is to review the analytical models of austenite transformations, taking into account the internal stresses obtained by various authors.

Research results

Stresses during heat treatment of steel products arise as a result of volumetric deformations associated with uneven temperature field and non-simultaneous occurrence of structural transformations. Moreover, the deformations caused by structural transitions are commensurate with temperature deformations.[23] The description of temperature and structural deformations is usually carried out with the help of a total linear expansion coefficient equal to:[3]

$$v_{\varepsilon} = d\varepsilon / dt \qquad (4)$$

where ε is free deformation, taking into account temperature and structural changes. The values of ε can be determined from the dilatogram3 of steel, depending on the structural composition, based on the additivity rule.[24] The studies[19–21] performed under isothermal conditions for uniaxial tension. It was established that plastic deformation of the order of 20 ... 30% significantly reduces the incubation period and increases the rate of perlite transformation. The process of acceleration during the deformation itself is characteristic of the bainite transformation, and when the load is removed, the transformation speed quite quickly decreases to its "normal" value. Thus, the determining factor in the acceleration of the bainitic transformation is the effective stress.[19] Plastic deformation associated with loading has a much smaller effect and cannot be attributed to accelerating factors. The maximum rate of bainitic transformation in the unloaded state occurs in the middle of the process, however, an increase in the rate of austenite decomposition at the initial stages of the process is characteristic of transformation under load.[20] This fact is explained by the acceleration of the restructuring of the crystal lattice under stress, which in turn leads to a decrease in the duration of the diffusion processes of redistribution of carbon required for the course of the transformation, and, consequently, to a slower response in the final stages. This also explains the decrease in the limiting degree of austenite decomposition with increasing load. The article[19] noted that the dependence of the kinetic parameters of the bainitic transformation on the effective voltage should be "strong" (exponential). The study of martensitic transformation[23] showed that the applied tension raises the temperature of the onset of transformation and accelerates the process at the initial stage. Subsequently, the transformation proceeds less intensively and ends at a temperature lower than in the unloaded state. The type of loading (tensile or torsion) has practically no effect on the results obtained.

The content of residual austenite increases with increasing load.[22] These facts indicate a similar nature of the effect of stresses on the bainite and martensitic transformations, which is explained by the same (shear) mechanism of transformations. Pearlite transformation, which is a diffusion process, reacts to external stress differently and much weaker.[20] When studying the effect of all-round compression on the course of non-martensitic transformations in hypoeutectoid steels, a slowing-down effect was determined. A mathematical model of steel hardening was proposed in[25] taking into account the effect of stresses on pearlite and martensitic transformations. To describe the pearlite transformation under non-isothermal conditions, the theory of isokinetic reactions was used.[9] It is accepted that the course of the pearlite transformation depends on the average stress. When describing the isothermal kinetics by the equation Avrami (1), it was proposed to replace the coefficient K with the following expression:

$$\kappa_{a=\kappa(t)}{}^{exp(nc\sigma_0)} \qquad (5)$$

where σ_0 is the average stress;[26] c - experimentally found coefficient, t - steel temperature. For martensitic transformation, the dependence on the stress intensity is accepted:

$$V_m = (1 - Vp)\{1 - exp[-a(m_s - t + b\sigma_i)]\} \qquad (6)$$

where σi is the stress intensity[26] a, b - constants obtained experimentally. In[27] the described approach was generalized to the case of the successive decomposition of austenite in the pearlite, bainite, and martensitic regions. In mathematical modeling of pearlite and bainite transformations, formulas similar to those obtained in[28] for bainite transformation without a load were used under the assumption of an additive course of the process. The volume fraction of perlite in an arbitrary cooling mode, taking into account the dependence (5) is determined by the formula:

$$V = 1 - \exp[-\{\int_{\tau}^{\tau} K_p(\mathrm{t})^{1/a} \exp(\mathrm{c}_{p\sigma_0})d\tau\}^a] \qquad (7)$$

For account the volume fraction of bainite used a more complex expression:

$$V = (1 - V_b)\,\mathrm{m}\exp[-\{\int_{\tau}^{\tau} K_p(\mathrm{t})^{1/a} \exp(\mathrm{c}_{p\sigma_0})d\tau\}^a] \qquad (8)$$

The factor m makes it possible to take into account the presence in many alloyed steels of the limiting degree of bainite transformation, which at given temperatures and the stress-strain state cannot be exceeded with increasing duration of the process. The value of m is calculated by the formula:

$$m = (\mathrm{B}_s - t + a_B\sigma_0 + b_i\sigma_i + g_B\varepsilon_i^p)d \qquad (9)$$

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where B_s is the onset temperature of the bainitic transformation in steel not subjected to mechanical stress; ε_i^p is the intensity of plastic deformations;[26] $\grave{a}_B$, $b_{\mathbf{i}}$, g_B, d - empirical constants.

For martensitic transformation, the following equation was used:[29]

$$Vm = (1 - V_P - V_B)\{1 - exp[-a(M_s - t + a_M\sigma_0 + b^i M\sigma_i gM\varepsilon_i^p)] \quad (10)$$

where a_M, $b^i{}_M$, g_M, a are empirical constants. Due to the lack of experimental data to determine the numerous parameters of the mathematical model, the values of the part of the constants are set equal to zero, others are approximately taken in.[18] Calculations were made for quenching bainite in water of cylindrical parts with a diameter of 1 m with varying constants. In the course of a numerical experiment, a significant dependence of the determined structural composition on the task of the constants was revealed. The basic assumption of work, which consists in the fact that the displacement of the field of bainitic transformations of TTT diagrams described in the same way as for pearlitic, by relation (5), is hardly justified. The bainitic transformation, as well as the martensitic, has a shear character[20] and therefore for him, as for the martensitic transformation,[25] it is advisable to accept the dependence of the kinetic parameters of the process on the stress intensity. Such an assumption was made in[30] in which the shift of the ITD under the action of a complex stress state was carried out according to the dependences obtained for simple stretching by replacing σ with σ_i. In addition to this drawback, it should be noted that multiplying the expression in curly brackets of equation (8) by the value of m, depending on temperature, leads to a violation of the additivity rule (Shayl's rule) determined by the condition:[31]

$$\int_{\tau_1}^{\tau_2} \frac{d\tau}{\tau_v(\mathrm{t})} = 1 \qquad (11)$$

where $\tau_V\,(t)$ is the time of isothermal achievement of the degree of conversion V at temperature t; τ_2- τ_1 is the time to reach in the non-isothermal process. The authors of article[32] when studying the acceleration of martensitic transformation under the action of tensile stresses occurring at negative temperatures in nickel-chromium steels, suggested that the decay kinetics depends on both the average stress and the stress intensity. In[33] an expression was theoretically found that establishes the effect of the stress level in the γ-phase on the martensite formation rate dn_α/dt:

$$dn_\alpha / dt = (L_{11}\Delta\phi + L_{12}\sigma_\gamma)e^{-\frac{v}{L}t} \qquad (12)$$

where $\Delta\varphi$ is the thermodynamic force for iron is the change in the chemical potential during the transition of particles from the γ-phase to the α-phase, σ_γ is the stress in the γ-phase; L_{11} and L_{12} are coefficients depending on the transformation temperature; v is the propagation velocity of microstrain in the sample (~ 1000m/s); L is the characteristic distance over which the shear microdeformation extends (the size of martensitic plates). At the initial stage of the formation of a shear structure, it is of the order of the diameter of the austenitic grain (~ 100μm), and then decreases with decreasing temperature.[33] Integrating the rate of formation of martensite, defined by formula (12) at a constant temperature and time from 0 to ∞, we obtain the following simple theoretical expression for calculating the amount of martensite produced depending on the stress in the γ-phase:

$$n_\alpha = n_{\alpha 0} + L_{12}\sigma_\gamma \qquad (13)$$

where $n_{\alpha 0}$ is the amount of martensite that is formed in the absence of stresses in the γ-phase. This quantity can be calculated using the Coetin – Marburger formula,[34] or using the more accurate formula proposed in:[35]

$$n_{\alpha 0} = A_m\left(1 - \exp\left(-K_\alpha \frac{M_s - T}{T - M_f}\right)\right) \qquad (14)$$

where A_m is the amount of austenite that has survived to M_s;

M_s is the temperature of the onset of the formation of martensite;

M_f is the temperature of the end of the formation of martensite;

K_α is the coefficient characterizing the rate of formation of martensite near the temperature M_s.

Accounting for the stress acting in the γ-phase according to expressions (13) and (14) leads to an increase in the temperature of the end of the formation of martensite M_f. Nevertheless, the experimental data accumulated to date do not allow to reliably describe the effect of the stress state on structural transitions during heat treatment of steels for the hot deformation tool. The study of this effect is especially convenient to carry out in isothermal conditions under uniaxial tension. To reliably predict the structural state of steels during hot deformation and heat treatment, it is necessary to conduct a comprehensive study related to the experimental study of the effect of stresses on the transformations of all types and the creation of an adequate mathematical model of austenite decomposition based on the experimental data obtained, taking into account this effect.

Conclusion

I. The analysis of the presented works shows that mathematical modeling of austenite decomposition during heat treatment is possible using both TTT and CCT diagrams. In the first case, the use of kinetic models is preferable. In the second, it is advisable to apply the theory of isokinetic reactions. In this case, the effect of the stress-strain state arising in the process of heat treatment of parts on the kinetics of structural transformations is usually not taken into account.

II. The experimental data accumulated to date do not reliably describe the effect of the stress state on structural transitions during the heat treatment of steels.

III. A simple theoretical expression is proposed for calculating the amount of martensite formed as a function of the stress in the γ-phase.

IV. To reliably predict the structural state of steels during hot deformation and heat treatment, it is necessary to conduct a comprehensive study related to the experimental study of the effect of stresses on the transformations of all types and the creation of an adequate mathematical model of austenite decomposition based on the experimental data obtained, taking into account this effect.

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Conflicts of interest

Authors declare that there is no conflict of interest.

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