Chapter 3

MODELS OF STRUCTURAL PHASE TRANSFORMATIONS AND MECHANICAL PROPERTIES OF ALLOY STEELS ROLLS

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ABSTRACT

Temperature relation of interlamellar spacing of pearlite, with the supercooling in carbon steels, based on previously theoretically foundation has been determined by the pearlite and bainite phase volumes in the alloy steels from the degree of supercooling. Calculated data corresponds to the experimental results with a sufficient accuracy. Development of a diffusion model of discontinuous transformation of austenite makes possible to theoretically explain formation of bainitic ferrite in low carbon steel in the same temperature range. These models

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are applied to the study of multi-stage heat treatment of large-scale rolls. Adapted analytical models are applied to the calculation of structural phase transformations and mechanical properties with the finite-element models of rolls. Results show structural phase components in the special alloy steels 50CrMnMoV, 45Cr3MnNiMoV at different stages of the rolls manufacturing process.

**Keywords:** alloy steel, heat treatment, phase transformation, finite-element model, rolls

**INTRODUCTION**

Improvement of heat treatment process is efficient. Complete picture is known by the main features and characteristics of processed alloys. Kinetics of supercooled austenite transformation, on which the basis issues are addressed of hardenability, heat treatment schedules mechanical properties (YTS, UTS, E% and HB).

Experimental study of microstructure components in the heat treatment of alloy steels consists of time-temperature (TTT) and continuous cooling (CCT) transformation diagrams, as well as steels hardenability. The use of numerous experimental tests studying the transformation phases are especially limited for large-scale parts. Isothermal TTT diagrams are used only for qualitative assessment of the effect of chemical composition on the process of austenite decomposition. The CCT diagrams can’t provide reliable information of the steel microstructure, when industrial cooling schedule differs from the cooling conditions during experiments. That is why, CCT diagrams are only used to quantify the stability of the austenite under continuous cooling process. Hardenability makes it possible to predict the structure of steel after heat treatment, based on its chemical composition, which is characteristic of only a particular grade of steel. Limitations, associated with this method of experimental data presentation, can be eliminated by creating analytical and finite element mathematical models, whose parameters are determined from the abovementioned experimental methods.
The most fundamental results in the modelling of phase transformation kinetics were obtained in works of A. N. Kolmogorov, M. Avrami, W. A. Johnson and R. F. Mehl [1, 2, 3]. The basic model known as JMAK (Johnson–Mehl–Avrami–Kolmogorov) is still widely used with its modifications, where the volume of the newly formed phase is supposed to be dependent on the probability of nucleation centres. The linear speed of growth and the elapsed time.

Fundamental review of mathematical modelling of phase transformation process was performed by J. W. Christian [4]. In this book, it is indicated that the analytical models do not take into account the clearly non-stationary nucleation process, which is contrary to the real conditions.

Any variations of microstructure cause change of mechanical properties of the materials, therefore models were used of grains growth and refinement [5] during dynamic and static recrystallization, based on C. M. Sellars equation [6] that can significantly improve metal flow patterns under plastic deformations.

Modern researches are implemented in the specific software applications, like JMatPro or ESI Group products for steels modelling. User is able to calculate phase changes for an assigned chemical composition of steel and different modes of treatment, e.g., continuous heating and tempering. That makes it possible to predict micro structure after heat treatment [7-9], including large-scale rolls [10-12]. However, the possibility of universal FEM software in nonlinear thermo-mechanical models calculation, running with different properties every time, is limited to the analysis of special alloy steels used for rolls manufacturing. User has to integrate own routines for calculating diagrams of phase transformations. For example, heat treatment is combined with cryogenic processing [13]. This opportunity can provide only advanced software products like QForm, DEFORM or MSC. Marc due to embedded interface for external user modules inclusion.

The main goal of this work is construction of analytical models of structural phase transformations and properties in carbon steels and their application to the modeling of the microstructure and mechanical properties of roll steels. Simulations of multi-stage heat treatment are
conducted in accordance with technological schedules of the rolls manufacturer [14], namely, stages of spray quenching and differential heat treatment (DHT). It was necessary to determine the ratio of phase components in the hardened layer of rolls (50-100 mm) for alloy steels 50CrMnMoV and 45Cr3MnNiMoV.

**DIFFUSION MODELS OF AUSTENITE TRANSFORMATION**

One of the most important diffusion transformations in iron-carbon alloys is the eutectoid transformation of austenite.

Zener suggested ratio for interlamellar spacing as a function of the steel supercooling value $S_0 \sim \Delta T^{-1}$ [15]. Experimental results show, however, that the measured values of the interlamellar spacing of pearlite significantly greater of those values, which gives the Zener’s model [4, 16, 17].

An important kinetic characteristic of austenite transformation process is the rate of growth of pearlite $V$. The value of growth rate was obtained by R. F. Mehl in the form: $V = K S_0$, where $S_0$ is the interlamellar spacing; $K$ – coefficient of proportionality, for which you need to solve a differential equation of the stationary growth of pearlite [4, 16, 18].

With such models, it is impossible to reach an equilibrium redistribution of the components in the pearlite; however, it is possible to calculate the growth rate and degree of redistribution of the components [16]. This requires another physical principle to describe it.

In the work [19] as this principle was used the law of energy conservation (balance of heat) during the transformation of austenite and the diffusion balance of the carbon. The result is a characteristic equation with a variable thickness of pearlite $\Delta = S_0/2$, whose solution makes it possible to find the dependence for $\Delta$ and for the growth rate of pearlite $V = K \Delta T \exp(-Q/2RT)$. It is significantly different from that obtained by the Zener expression for the growth rate of pearlite based on considerations of dimensionality and some physical-chemical principles:
V~ΔT² exp(-Q/RT).

The authors of works [19, 20] found theoretically the dependence of interlammelar spacing of pearlite on the temperature of supercooling of the alloy in the form of $S_0 \sim \sqrt{D_x/\Delta T}$ with the corresponding experimental data.

In work [21], it was developed a diffusion model of discontinuous transformation of austenite, which made possible theoretically to explain joint formation of pearlite and bainitic ferrite in low carbon steel in the same temperature range.

In work [22], it have been developed a diffusion model of austenite transformation in carbon steel of eutectoid composition. Dependence of the pearlite growth rate and the interlammelar spacing $S_0$ on the supercooling value shown on Figure 1 and Figure 2.

![Figure 1. Dependence of the pearlite growth rate $V_p$ on the supercooling value $\Delta T$: $V_{p1}$ – calculated by formula (34) in work [22]; $V_{p2}$ – by Zener's formula [15, 16].](image-url)
Figure 2. Dependence of the interlammelar spacing $S_0$ on the degree of supercooling $\Delta T$ of the alloy (– the experimental data from [23], p. 122).

**ANALYTICAL MODELS OF STRUCTURAL PHASE TRANSFORMATIONS**

Analytical model of austenite transformation was applied for the steel structure modelling based on the results obtained in [13, 19, 20]. The M. Avrami equation was used of the phase transformation kinetics, written in the following form:

$$P_\alpha = 1 - \exp\left(-\left(V\tau\right)^n\right),$$

where $P_\alpha$ = result of the phase transformation (amount of formed pearlite or bainite); $V$ = relative rate of transformation; $n$ = degree of equation; $\tau$ = time of transformation (below critical point $Ac_1$ for the pearlite and $Ac_0$ for bainite).

The relative rate of conversion is given by [19, 20]:

$$V = K \cdot \Delta T \exp\left(-Q/2RT\right),$$

(2)
where $\Delta T = T_c - T$, $T$ – current temperature; $T_c$ – temperature critical points of transformation $A_{c1}$ or $A_{c0}$; $Q$ – the activation energy of carbon diffusion in the alloy steel; $K$ – constant coefficient; $R$ – universal gas constant, 1.987 [cal K$^{-1}$ mol$^{-1}$]. Parameter $Q$ for pearlite is equal to the activation energy of carbon diffusion in the austenite of steel, and for bainite, it is equal to the activation energy of carbon diffusion in steel ferrite. Temperature $A_{c0}$ for roll steels is calculated from the condition that the maximum of the bainite growth rate coincides according to temperature, calculated from equation (2) and its experimental value on an isothermal diagram. This value is 500°C for steel 50CrMnMoV and 380°C for steel 45Cr3MnNiMoV.

Equation (2) describes the temperature dependence of the growth rate of transformation products in cooling steel with a maximum at certain supercooling temperature $\Delta T$ determined on the charts of isothermal transformation of austenite. This relation gives the experimental value of the diffusion activation energy $Q$. The steel used for model verification is 65Cr2Si3MoV with known diagrams of austenite transformation and the structure after treatment.

The exponent of the kinetic equation for the pearlite and bainite transformation is given by the formula [23]:

$$n = \frac{1.7665}{\lg(\tau_{95\%}) - \lg(\tau_{5\%})},$$

(3)

where $\tau_{5\%}$ – the least time of 5% phase formation; $\tau_{95\%}$ – the least time of 95% phase formation. These times are determined from TTT and CCT diagrams of austenite transformation for each phase (pearlite or bainite). The maximum transformation rate was calculated using the formula:

$$V_{\max} = \sqrt{0.0513 / \tau_{5\%}}$$

(4)

Based on this value $V_{\max}$, the coefficient $K$ is determined in formula (2).
The amount of martensite formed in the steel can be calculated from the following equation, proposed by the authors in [13]:

\[ P_a = A_m (1 - \exp \left( -K_a \frac{M_s - T}{T - M_f} \right)), \]  

(5)

where \( A_m \) – the amount of austenite retained to \( M_s \) temperature; \( M_s \) – temperature of the start of martensite transformation; \( M_f \) – temperature of the end of martensite transformation, \( K_a \) – coefficient of martensite formation rate at the temperature \( M_s \).

The improved model explicitly contains the rate of phase and structure transformation (ferrite, pearlite, bainite) that allows more clearly to interpret physical coefficients. To describe the process of martensite formation, the model includes both the start and end temperature of transformation.

**CALCULATION OF MECHANICAL PROPERTIES OF STEELS**

Predicted yield strength of carbon steel is calculated by the formula:

\[ \sigma = \sigma_F P_F + \sigma_P P_P + \sigma_B P_B + \sigma_M P_M, \]  

(6)

where \( \sigma_F, \sigma_P, \sigma_B, \sigma_M \) - respectively yield strength of ferrite, pearlite, bainite and martensite, MPa; \( P_F, P_P, P_B, P_M \) – fractions of structural components.

*Strength of ferrite:*

\[ \sigma_F = \sigma_0 + \sum k_i C_i, \]  

(7)

where \( \sigma_0 \) – initial strength, MPa; \( C_i \) - content of alloy elements (%); \( k_i \) – coefficients of alloy elements contribution into steel strength.

*Strength of pearlite:*

\[ \sigma_p = \sigma_F + \frac{K_p}{\sqrt{s}}, \]  

(8)
where \( S = S_0 / \sqrt{V_p} \) - interlamellar spacing of pearlite; \( S_0 \) – initial value; \( K_p \) - empirical coefficient, MPa; \( V_p \) – cooling rate in pearlite region.

**Strength of bainite:**

\[
\sigma_B = \sigma_{F+P} + \left( \frac{B_s - T_i}{B_s - M_s} (\sigma_M - \sigma_{F+P}) \cdot \Delta P_B \right) / P_B ,
\]

(9)

where \( \sigma_{F+P} \) – strength of ferrite-pearlite composition; \( B_s, M_s \) – temperatures of starting points of bainite and martensite transformations; \( T_i \) – temperature of bainite transformation at the \( i \)-th time step; \( \Delta P_B \) – bainite fraction increasing within time step; \( P_B \) – fraction of bainite.

**Strength of martensite:**

\[
\sigma_M = \sigma_F + \frac{K_M}{L} ,
\]

(10)

where \( L = L_0 / \sqrt{V_M} \) - the average length of the slip plane of martensite; \( L_0 \) – initial value; \( K_M \) - empirical coefficient, MPa; \( V_M \) – cooling rate in martensite region. In theory, cooling rates at different regions should be equal: \( V_p = V_M = V_{const} \), but their real difference is accounted in the calculations.

The analytical relationship of steel hardness and yield strength of structural components is described by the following formula:

\[
HRC = \sqrt{K_p \sigma_p P_p + K_B \sigma_B P_B + K_M \sigma_M P_M}
\]

(11)

The adequacy of this model depends on how accurately the mechanical properties of microstructure components are determined by microhardness measurements. Although Hall-Petch effect is not directly accounted in the model, grain size influence is taken into account by some geometrical parameters of microstructure: interlamellar spacing of pearlite and average length of the slip plane of martensite.
A Technique for Simulation of Structural Phase Transformations in Rolls

The large-scale backup rolls for modern hot and cold rolling mills are up to 2000 mm in diameter and of 50 t weight. The main mechanical properties of rolls include the following parameters: required microstructure (tempered troostite with uniformly distributed carbides) through the whole depth of hardened layer (70-80 mm), hardness 55-65 HSD with variation 2-3 HSD, tensile strength 1200-1400 MPa. Special alloy steels 50CrMnMoV, 45Cr3MnNiMoV are used for the work rolls and backup rolls production respectively. The chemical composition of roll steels are given in Table 1.

<table>
<thead>
<tr>
<th>Steels</th>
<th>Chemical composition, %</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>C</td>
</tr>
<tr>
<td>50CrMnMoV</td>
<td>0.59</td>
</tr>
<tr>
<td>45Cr3MnNiMoV</td>
<td>0.45</td>
</tr>
</tbody>
</table>

Strict requirements to rolls quality are mainly satisfied due to multistage heat treatment process, which lasts up to several days. Sampling of rolls barrels for microstructure testing is almost unavailable. Therefore, mathematical model is implemented to calculate temperature and stresses. Actually, FEM modelling (Figure 3) is practically the only way to get additional information inside the rolls for the quenching control of newly developed steels and schedules including deep cryogenic treatment for high-chromium steels. However, such models should account phase transformations to be adequate to reality that have certain issues.

Based on the changes in the yield limit of the roll material, it can be argued that the maximum voltage does not exceed 1120 MPa yield strength at the end of 2nd stage, however, are close to the value of inelastic deformation. Therefore, they should not increase the intensity of the roll
cooling and reduced, but at the same time increase the quenching on the 1st or the 2nd stage.

The analytical equation of phase transformations was adopted to be applicable in the FEM modelling. The developed analytical model along with the TTT and CCT diagrams of austenite decomposition is used to analyse the structure of alloy steels 50CrMnMoV and 45Cr3MnNiMoV.

The algorithm for modeling phase transformations in rolls of alloy steels is as follows.

1) Developing the FEM model from the rolls drawings.
2) Modeling of temperature and stresses over the roll volume.
3) Calculation of critical points of phase transformations according to the regression model developed for certain range of chemical compositions of alloy steels.

4) Building of TTT for the calculated critical points.

5) Construction of a CCT by the proposed calculation method.

6) Matching the temperature curves over the roll barrel depth with the CCT diagram.

7) Calculation the boundaries of phase transformations from the cooling curves at different depths of roll and their comparison with the points of the CCT.

8) Calculation the number and fractions of microstructure components in the steel at a given depth after the end of cooling.

The analytical TTT and CCT diagrams are currently determined for a given range of chemical composition of rolls by the statistical processing of the highly alloyed steel grades. That is resulted in a possibility to take into account the complete list of alloying elements and enough wide range of their mass fraction. This is the advantage of the developed analytical models in contrast to the experimental methods of the TTT and CCT determination by the dilatometric measurements.

**STUDIES OF ROLL STEELS ON MODELS**

In steel 50CrMnMoV (Figure 2a) there is practically no temperature range of austenite stability between the areas of pearlite and bainite, which formation begins earlier than in 45Cr3MnNiMoV steel.

Under isothermal conditions, alloy steel 45Cr3MnNiMoV undergoes two transformations: pearlitic and bainitic (Figure 2b) between which an area exists of increased stability of austenite in the temperature range 350-450°C. The region of pearlite transformation is shifted to the right side, which indicates an increased stability of austenite due to alloying elements.
Differences in alloy elements of these steels determine the type of diagrams (Figure 3). The steel structure 50CrMnMoV cooled at a rate 0.24°C/s (corresponds to roll depth 80 mm) has at 20°C pearlite (93%) and bainite (7%). Steel 45Cr3MnNiMoV cooled at a rate 0.24°C/s includes at room temperature bainite (48%), martensite (47%) and retained austenite (5%).

The calculated CCT of steel 50CrMnMoV has an intersection of bainite and pearlite regions at the temperature at 400°C, where these microstructure components are formed simultaneously (Figure 3a). The areas of pearlitic and bainitic transformations for 45Cr3MnNiMoV steel (Figure 3b) are shifted to the region of lower cooling rates compared to steel 50CrMnMoV.

Thus, the working layer of the roll at a depth of 80 mm has quenching microstructure components that provide high hardness of rolls at this depth (more than 50 HRC). The depth of rolls hardenability is assumed as the distance from the roll surface where not less than 50% of bainite and martensite are formed for this cooling rate.

![Figure 4. TTT diagrams of alloy steels: (a) 50CrMnMoV (Ac$_3$ = 810°C, Ac$_1$ = 757°C, Ms = 250°C); (b) 45Cr3MnNiMoV (Ac$_3$ = 815°C, Ac$_1$ = 720°C, Ms = 300°C).](image-url)
the distance from the roll surface where not less than 50% of bainite and martensite are formed for this cooling rate.

![Diagram of phases in 50CrMnMoV steel](image-a)

![Diagram of phases in 45Cr3MnNiMoV steel](image-b)

Figure 5. Diagrams of phases in steels 50CrMnMoV (a) and 45Cr3MnNiMoV (b) depending on the cooling rate (P – pearlite; B – bainite; M – martensite).

The calculations for the 50CrMnMoV and 45Cr3MnNiMoV steels are given in Figure 5 and 6 with roll temperatures at a depth of 0...200 mm (with increment of 20 mm). Results are obtained by the finite element model for the applicable modes of spray quenching. These graphs also contain the $\text{Ac}_3$, $\text{Ac}_1$, $\text{Ms}$, calculated points bainite (B1, B2) transformations and regions of pearlite (P1, P2) and bainite (B1, B2) transformations from the building CCT diagrams.
CALCULATION OF MECHANICAL PROPERTIES OF STEEL 50CrMnMoV AND 45Cr3MnNiMoV

The depth of rolls hardenability is assumed as the distance from the barrel surface where not less than 50% of bainite and martensite are formed for certain cooling rate. At the depth of hardened layer, rolls should have quenching microstructure and hardness about 50 HRC.

Calculated relationships of tensile strength and hardness depending on cooling rate for alloy steels 50CrNiMoV and 45Cr3MnNiMoV are given in Figure 7. Natural increasing of steels strength and hardness with higher cooling rates is obviously visible on these graphs.
Figure 7. Calculated relationships of tensile strength (a) and hardness (b) depending on cooling rate for alloy steels 50CrNiMoV and 45Cr3MnNiMoV.

The hardness and strength of 45Cr3MnNiMoV steel in the entire range of cooling rates is higher than that of steel 50CrNiMoV. To ensure a hardness of more than 50 HRC, the steel 50CrNiMoV needs to be cooled at a rate of more than 2.0°C/s.

**ANALYSIS OF HEAT TREATMENT OF ROLLS MADE OF STEEL 50CrMnMoV**

Figure 8. Calculations of spray quenching for work roll of 50CrMnMoV steel.

The calculations for the 50CrMnMoV and 45Cr3MnNiMoV steels are given in Figure 5 and 6 with roll temperatures at a depth of 0...200 mm (with increment of 20 mm). Results are obtained by the finite element
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model for the applicable modes of spray quenching. These graphs also contain the Ac3, Ac1, Ms calculated points bainite (B1, B2) transformations and regions of pearlite (P1, P2) and bainite (B1, B2) transformations from the building CCT diagrams.

During spray quenching (I stage 0...600 s; II stage 600...1200 s) the formation of bainite is only on the surface of the roll, and perhaps to a depth of 10 mm. At a depth of 20...200 mm, the temperature is the pearlite (P1, P2) region. After termination of the cooling (2400 s) and subsequent self-heating from internal layers, roll temperature converges to an average value of about 600°C, thus bypassing the bainite region up to a depth of 120 mm and providing pearlite structure at that depth.

ANALYSIS OF HEAT TREATMENT OF ROLLS MADE OF STEEL 45Cr3MnNiMoV

In the process of spray quenching (I stage 0...600 s; II stage 600...1200 s) martensite region (below Ms line) is not captured even on the roll surface. Within the whole depth of 200 mm the temperature is in the regions bainite (B1, B2) transformations. After termination of the cooling (2400 s) and subsequent self-heating from internal layers, roll temperature converges to an average value of about 600°C, slightly higher than the desired tempering temperature (500°C), thus bypassing the bainite region. Subsequent heating of the roll takes place entering the pearlite region at a depth of 20...200 mm.

The modelling of phase transformation is based on calculated CCT and TTT diagrams of 50Cr5NiMoV and 45Cr3MnNiMoV steels. Results of modelling showed their conformity by final phase composition with the experimental data. The real trajectories of cooling and rates at different points do not provide quenching structure (bainite, martensite) in the whole depth of backup rolls barrel (70 mm). For steel 50Cr5NiMoV, bainite structure is only possible in a thin surface layer (10 mm) due to self-heating from internal layers. It was recommended to increase the cooling
time of the rolls at the spray-hardening machine for achieving lower temperatures at the desired depth of the roll.

Figure 9. Calculations of spray quenching for backup rolls of 45Cr3MnNiMoV steel.

CONCLUSION

In this work, data are presented on the diffusion model of austenite transformation developed earlier. The analytical dependencies of this model were applied to the calculation of pearlitic and bainitic transformations in carbon and roll steels. When calculating the parameters of pearlitic and bainitic transformations for roll steels, it was established that the activation energy of carbon $Q$ for pearlite is equal to the activation energy of carbon diffusion in the austenite of steel, and for bainite is equal to the activation energy of carbon diffusion in steel ferrite. To calculate the amount of martensite, the authors proposed a new equation that has been used in this work.

The technique is improved for determining the phase composition of steels in the quenching process, allowing the calculation of the structural components volumes in the steel at any time along the actual cooling trajectory at any point of the roll obtained by the finite element model.

Based on the developed model, isothermal and structural diagrams for 50CrMnMoV and 45Cr3MnNiMoV steels have been constructed; their correspondence to experimental data has been established. The analysis is
performed of the spray quenching of rolls of alloy steels 50CrMnMoV and 45Cr3MnNiMoV, according to the existing heat treatment schedules in the rolls production.

For work roll of steel 50CrMnMoV, it is possible to obtain a bainitic structure only in a thin (up to 10 mm) near-surface layer. Corrections of heat treatment schedule were proposed. While for the backup rolls of steel 45Cr3MnNiMoV, the quenching hardness and bainite with martensite structure is achieved through the whole depth of working layer (up to 200 mm).

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