MODELING MECHANICAL PROPERTIES OF STEELS WITH COMPLEX MICROSTUCTURE

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Abstract

Mathematical models of the mechanical properties for steels with a complex microstructure are presented. These models are a component of a recently developed integral hot rolling model for mill 2000 of SEVERSTAL (STAN 2000), along with the models for predicting austenite microstructure evolution under hot rolling and its transformation during subsequent cooling. The models for predicting yield and tensile stresses are based on the rule of mixture according to which the contributions of individual structural components are proportional to their volume fractions. The following structural components are considered: polygonal ferrite, pearlite, bainite of different morphology, and martensite. The ferrite grain size contribution is described using the Hall-Petch equation. Pearlite contribution is calculated taking into account the combined effect of its volume fraction and inter-lamellar distance. Bainite contribution to strength properties is determined taking into account the size of bainite blocks, volume fractions of bainites with different morphology and dislocation density. Martensite contribution is defined with account of its volume fraction. For the micro-alloyed steel grades, additional hardening caused by the Nb(C,N) and V(C,N) precipitates formed at the hot rolling stage is taken into account. The models were calibrated using experimental data base on mechanical properties for a number of steel grades rolled on mill 2000 of SEVERSTAL with chemical compositions covering the following ranges of alloying elements content: C(≤0.65); Mn(≤2.0); Si(≤1.0); Cr(≤0.9); Ni(≤0.6); Cu(≤0.5); Mo(≤0.4); Nb(≤0.05); V(≤0.065); Ti(≤0.06). The predicted mechanical properties are in good agreement with the experimental data.

Keywords: steels, microstructure, mechanical properties, modeling

1. INTRODUCTION

Substantial attention has been paid over the last decades to the development of integral mathematical models for predicting the microstructure and mechanical properties of hot rolled steels. During the time since the creation of the first such models [1,2], there has been a tendency to use more physically based models for describing the complicated processes of austenite microstructure evolution under hot rolling, as well as its transformation during subsequent accelerated cooling with formation of different structural components such as ferrite, pearlite, bainite and martensite. These models were used thanks to their higher ability to predict the complex effects of alloying. Creation of a new generation of integral hot rolling models is possible when using physically justified sub-models of the separate processes of structure formation based on reliable approaches to calculating the thermodynamic and kinetic process parameters with an accurate account of the alloying effects.

Recently, the authors developed an integral model of hot rolling for mill 2000 of SEVERSTAL (STAN 2000), which corresponds to the noted modern requirements [3]. Physically based mathematical models needed for a quantitative description of the austenite microstructure evolution during hot rolling (the models of austeniute grain growth, its dynamic and static recrystallization model coupled with the model of strain induced carbonitrides precipitation in microalloyed steels) were described elsewhere [4], as well as the model for austenite decomposition under accelerated cooling with formation of all practically important structural components [3,5].

The model for predicting final mechanical properties of steel on the basis of the calculated set of significant microstructure parameters is one of the important sub-models of the integral hot rolling model. A model for the mechanical properties estimation in modern steels with a complex microstructure is described in the present paper. This model is an important component of the developed integral model STAN 2000, and it was calibrated using a mechanical properties data base for a number of practically important steels hot rolled on mill 2000 under different rolling regimes.

2. MODELING OF MECHANICAL PROPERTIES

The models for yield (σ_Y) and tensile (σ_T) stresses calculation are based on the rule of mixture according to which the contributions of individual structural components are proportional to their volume fractions. The following structural components are considered: polygonal ferrite (PF), pearlite (PE), bainite (B) of different morphology and martensite (M). Mechanical properties are estimated using the equations:

$$\begin{aligned}\sigma_Y &= \sigma_0^Y + \Delta\sigma_{ss}^Y + \Delta\sigma_{PF}^Y + \Delta\sigma_{PE}^Y + \Delta\sigma_B^Y + \Delta\sigma_M^Y,\\ \sigma_T &= \sigma_0^T + \Delta\sigma_{ss}^T + \Delta\sigma_{PF}^T + \Delta\sigma_{PE}^T + \Delta\sigma_B^T + \Delta\sigma_M^T,\end{aligned} \quad (1)$$

$\sigma_0^{Y;T}$ are the base contributions; $\Delta\sigma_{ss}^{Y;T}$ are solid solution contributions; $\Delta\sigma_{PF}^{Y,T}$, $\Delta\sigma_{PE}^{Y;T}$, $\Delta\sigma_B^{Y;T}$, $\Delta\sigma_M^{Y;T}$ are contributions of the corresponding structural components (excluding base contribution and the contribution of the solid solution).

Relative elongation is calculated using the formula:

$$\delta = \delta_0 + \Delta\delta_{ss} + \Delta\delta_{PF} + \Delta\delta_{PE} + \Delta\delta_B + \Delta\delta_M, \quad (2)$$

δ_0 is the base value of elongation; $\Delta\delta_{ss}, \Delta\delta_F, \Delta\delta_{PE}, \Delta\delta_B, \Delta\delta_M$ are the contributions to reduction of the plasticity caused by corresponding hardening components of the material.

Calibration of the model for predicting mechanical properties was performed using an extensive experimental data base on the mechanical properties for 32 steel grades (**Table 1**) with a wide variation in chemical composition that were hot rolled on mill 2000 of SEVERSTAL under different regimes. Chemical compositions of the steels cover the following practically important ranges of alloying elements content: C(≤0.65); Mn(≤2.0); Si(≤1.0); Cr(≤0.9); Ni(≤0.6); Cu(≤0.5); Mo(≤0.4); Nb(≤0.08); V(≤0.09); Ti(≤0.07) (mass.%).

Table 1 Set of the steel grades hot rolled on mill 2000, for which the data on mechanical properties used for model calibration (unstressed designations of the steel grades represent designations adopted in Russia and recorded using the Cyrillic alphabet)

Low carbon steels	CHES01, 01ЮТ, DD11
Plane carbon steels	Ст.20, 08ПС, 20К, 20ПС, S235JR, Ст3СП, СТ0, Ст2ПС, 20Ю
Average carbon steels	25ГЮ, 45, 65Г
HSLA steels	09Г2С, 10ХСНД, 12ХМ
Microalloyed steels	09ГСФ, 20ГЮТ, 20-КСХ, D40S, X80, 17Г1С-У, X42, X52, К52, К56, 10Г2ФБ, S700, S355J2

In addition, we used the set of calculated values for the necessary parameters of microstructure of the given steels rolled under the according regimes. The values of the necessary parameters (volume fractions of the structural components, the average ferrite grain and bainite blocks sizes, characteristic transformation temperatures, volume fractions and sizes of carbonitrides in microalloyed steels) were calculated using the

computer model STAN 2000. The usable set of steels rolled at different regimes provides a wide range of microstructures, including both simple ferrite-pearlite and complex structures containing bainites of different morphology.

Description of the mathematical models under discussion, and the results we obtained from the models calibration are presented below.

For the base contributions, the following values were obtained: $\sigma_0^Y = 76$ МПа; $\sigma_0^T = 115$ МПа.

To calculate the solid solution hardening, the formula is evaluated which differs from the well-known one from literature [6] by the contributions provided by the silicon and manganese atoms:

$$\begin{aligned}\Delta\sigma_{ss}^Y &= 42w_{Mn} + 61w_{Si} + 15w_{Ni} + 39w_{Cu} + 11w_{Mo} + 80w_{Ti} + 678w_P + 1100w_N \text{ (MPa)},\\ \Delta\sigma_{ss}^T &= 46w_{Mn} + 83w_{Si} + 15w_{Ni} + 39w_{Cu} + 11w_{Mo} + 80w_{Ti} + 678w_P + 2800w_N \text{ (MPa)},\end{aligned} \quad (3)$$

w_X is the X alloying element concentration (mass. %).

When calculating the ferrite contribution into strength characteristics, the following formula is utilized:

$$\Delta\sigma_{PF}^{Y;T} = \left(K_{PF}^{Y;T} d_\alpha^{-0.5} + \sqrt{\left(\Delta\sigma_{PF_d}^{Y;T}\right)^2 + \left(\Delta\sigma_{Nb(CN)}^{Y;T}\right)^2 + \left(\Delta\sigma_{V(CN)}^{Y;T}\right)^2} \right) X_{PF} \text{ (MPa)}, \quad (4)$$

$K_{PF}^{Y;T} d_\alpha^{-0.5}$ is the ferrite grain boundaries contribution, calculated according with the Hall-Petch equation; d_α is an average volumetric ferrite grain size (mm); the second term in brackets represents the resulting contribution to the ferrite strengthening introduced by dislocations and corresponding carbonitrides particles formed in austenite at the stage of hot rolling; X_{PF} is ferrite volume fraction. The following values were obtained for the Hall-Petch coefficients: $K_{PF}^Y = 15.1$ MPa/мм$^{0.5}$; $K_{PF}^T = 17$ MPa/мм$^{0.5}$.

The following expression is used to calculate the contribution to the yield strength of ferrite caused by the dislocations, which are generated in this phase during austenite decomposition due to the intensive phase stresses:

$$\Delta\sigma_{PF_d}^Y = \begin{cases} 30\left[1 - \exp\left(-0.01\left(705 - \tilde{T}_{PF}\right)\right)\right] X_{PF} \text{(MPa)}, \text{ for } \tilde{T}_{PF} < 705 \\ 0, \text{ for } \tilde{T}_{PF} > 705 \end{cases} \quad (5)$$

$\tilde{T}_{PF}$ is the average temperature of the ferrite formation (°C). This contribution is not large due to the relatively low final density of dislocations in the ferrite, a significant proportion of which is annihilated due to rapid climb, accelerated with increasing temperature $\tilde{T}_{PF}$. When calculating the tensile stress of the ferrite, this dislocation contribution is not taken into account ($\Delta\sigma_{PF_d}^T = 0$).

The approach used to quantify the hardening contributions of the precipitate particles ($\Delta\sigma_{Nb(CN)}^{Y;T}$, $\Delta\sigma_{V(CN)}^{Y;T}$) is described in detail below.

Pearlite contribution is assessed taking into account the cumulative effect of its volume fraction and inter-lamellar distance, which decreases monotonically with decreasing pearlite formation temperature:

$$\begin{aligned}\Delta\sigma_{PE}^Y &= \left[140 + 0.55\exp\left(4000/\tilde{T}_{PE}\right)\right] X_{PE} \text{ (MPa)},\\ \Delta\sigma_{PE}^T &= \left[170 + 4.5\exp\left(3000/\tilde{T}_{PE}\right)\right] X_{PE} \text{ (MPa)},\end{aligned} \quad (6)$$

$\tilde{T}_{PE}$ is an average temperature of the pearlite formation (°C); X_{PE} is the pearlite volume fraction.

Calculating the contribution of bainite to the strength properties is performed with regard to their dependence on the bainitic blocks size, playing the role of an effective grain size in these structures [3]:

$$\Delta\sigma_B^{Y;T} = \sum_{i=1}^{3}\left(X_B^i\left(K_B^{Y;T}d_B^{-0.5} + \sqrt{\left(\Delta\sigma_{Bdi}^{Y;T}\right)^2 + \left(\Delta\sigma_{Nb(CN)}^{Y;T}\right)^2 + \left(\Delta\sigma_{V(CN)}^{Y;T}\right)^2}\right)\right)\,(\text{MPa}), \qquad (7)$$

X_B^i is the volume fraction of i-th bainite type (i = 1,2,3 corresponds to the granular and conventional bainite, and acircular ferrite, respectively [3]; d_B is an average volumetric size of the bainitic block (mm); $\Delta\sigma_{Bdi}^{Y;T}$ are strength contributions related with dislocations; $K_B^{Y;T}$ are the Hall-Petch coefficients for the bainitic microstructure which optimal values are found to be equal: $K_B^Y = 15$ MPa/мм$^{0.5}$; $K_B^T = 13$ MPa/мм$^{0.5}$.

In estimating contributions of the martensite, the following simplified formula is used:

$$\Delta\sigma_M^{Y;T} = \Delta\sigma_{M0}^{Y;T}X_M\,(\text{MPa}), \qquad (8)$$

X_M is the martensite volume fraction; appropriate values of the $\Delta\sigma_{M0}^Y$ and $\Delta\sigma_{M0}^T$ parameters are chosen to be equal 600 and 750 MPa, respectively.

Contribution of the dislocations into strength properties of bainites with different morphology is estimated as follows:

$$\Delta\sigma_{Bdi}^{Y;T} = \alpha_{di}^{Y;T}G_\alpha b\rho_{di}^{0.5}, \qquad (9)$$

$G_\alpha = 81\times10^9\,\text{Pa}$ is the shear modulus of the α-phase; $b = 2.5\times10^{-10}\,\text{m}$ is the modulus of the Burgers vector; ρ_{di} average dislocation density in bainite of i-th type (m^{-2}); $\alpha_{Bdi}^{Y,T}$ fitting parameters of the model (**Table 2**). Dislocation densities in bainites are estimated using the following formula [7]:

$$\log_{10}(\rho_{di}) = 9.2848 + \frac{6880.73}{\tilde{T}_i} - \frac{1780360}{\tilde{T}_i^2}, \qquad (10)$$

$\tilde{T}_i$ is the average temperature of i-th type bainite formation (°C).

Table 2 Resulting set of the optimal values of $\alpha_{Bdi}^{Y,T}$ parameters (for shortness the parameters dimensions are not presented)

$\alpha_{d1}^Y\times10^6$	$\alpha_{d2}^Y\times10^6$	$\alpha_{d3}^Y\times10^6$	$\alpha_{d1}^T\times10^6$	$\alpha_{d2}^T\times10^6$	$\alpha_{d3}^T\times10^6$
0.4	0.28	0.18	0.54	0.47	0.32

When calculating strengthening contributions caused by the carbonitrides particles, two mechanisms of overcoming them by moving dislocations were initially taken into account: 1) particles bowing (Orowan mechanism); 2) particles shearing. However, analysis has shown that we can restrict consideration only to the mechanism of bowing.

To calculate the stress level required for bowing $\Delta\sigma_b^{Y;T}$ the following well known expressions are used:

$$\Delta\sigma_{bj}^{Y;T} = \alpha_{bj}^{Y;T}\left[\frac{3.1G_\alpha b}{2\pi\left(\lambda_j - 2R_j\right)}\ln\left(\frac{\lambda_j - 2R_j}{4b}\right)\right]^{\psi_p};\quad \lambda_j = \sqrt{\frac{2\pi}{3f_j}}R_j, \qquad (11)$$

R_j, f_j are average radius and volume fraction of the j-type particles (j=1,2 correspond to Nb(C,N) and V(C,N) particles, respectively); λ_j is the average distance between j-type particles in the slip plane of the dislocations; $\alpha_{bj}^{Y;T}$ and ψ_p are model fitting parameters, the appropriate values of which were obtained to be equal: ψ_p = 0.6; α_{b1}^{Y} = 9.5; α_{b2}^{Y} = 8.3; α_{b1}^{T} = 7.8; α_{b2}^{T} = 6.9 (for shortness dimensions of these parameters are not presented). The following expressions for different contributions into elongation (%) calculated according with formula (2) are obtained:

$$\delta_0 = 54;$$

$$\Delta\delta_{ss} = -1.21\left(32w_{Mn} + 83w_{Si} + 15w_{Ni} + 39w_{Cu} + 11w_{Mo} + 80w_{Ti} + 678w_P + 5000w_N\right)^{0.5};$$

$$\Delta\delta_{PF} = -100.8X_{PF}d_{\alpha}^{0.5}; \qquad \Delta\delta_{PE} = -0.011X_{PE}\exp\left(5000/\tilde{T}_{PE}\right);$$

$$\Delta\delta_M = -34X_M;$$

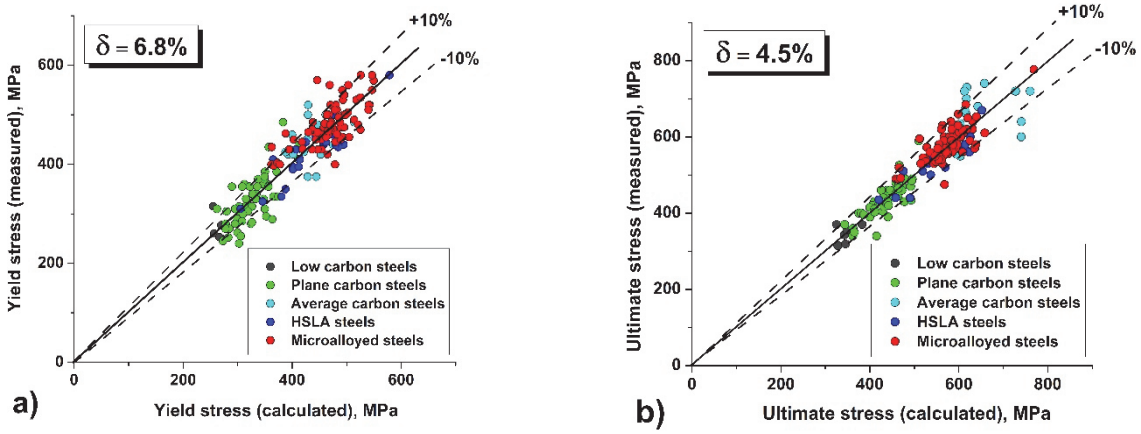
$$\Delta\delta_B = -50X_B d_B^{0.5} - \sum_{i=1}^{3} X_B^i \sqrt{\left(\Delta\delta_{B_{di}}\right)^2 + \left(\Delta\delta_{Nb(CN)}\right)^2 + \left(\Delta\delta_{V(CN)}\right)^2}, \qquad (12)$$

$$\Delta\delta_{B_{di}} = \alpha_{di}^E G_\alpha b \rho_{di}^{0.5}; \quad \alpha_{d1}^E = 0.17\times10^{-7}, \alpha_{d2}^E = 0.21\times10^{-7}, \alpha_{d3}^E = 0.2\times10^{-7};$$

$$\Delta\delta_j = \alpha_j^E \left[\frac{3.1G_\alpha b}{2\pi\left(\lambda_j - 2R_j\right)}\ln\left(\frac{\lambda_j - 2R_j}{4b}\right)\right]^{0.6}; \quad \alpha_1^E = 0.21, \quad \alpha_2^E = 0.3,$$

j=1,2 correspond to Nb(C,N) and V(C,N) particles, respectively.

Fig. 1 shows a comparison of the predicted and measured mechanical properties values for the investigated steels (**Table 1**).



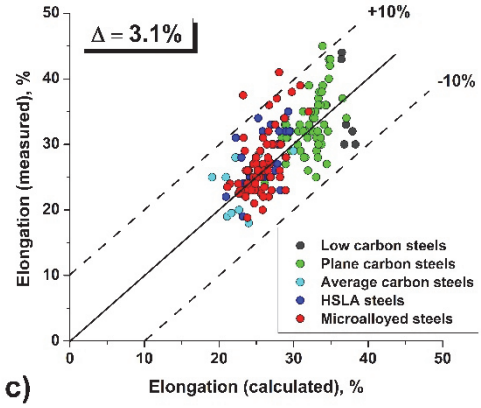


Fig. 1 Comparison of the calculated and measured yield stress (a), ultimate stress (b) and relative elongation (c) for the steels hot rolled on mill 2000 of SEVERSTAL (**Table 1**). δ and Δ are, correspondently, average values of the relative and absolute accuracy.

SUMMARY

This paper describes a mathematical model for estimating mechanical properties in modern steels with a complex microstructure. This model is an important component of a recently developed integral hot rolling model for mill 2000 of SEVERSTAL (STAN 2000). The model is calibrated using a mechanical properties data base for a number of practically important steels hot rolled on mill 2000 under different rolling regimes. In addition, we used the set of calculated values for the necessary parameters of microstructure of the given steels rolled under the according regimes. The values of the necessary parameters (volume fractions of the structural components, the average ferrite grain and bainite block sizes, characteristic transformation temperatures, volume fractions and sizes of carbonitrides in microalloyed steels) were calculated using the computer model STAN 2000. Predictions of the mechanical properties are compared with experimental data and show a good agreement.

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