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Regression Relations for Estimating the Mechanical Properties of Steels Subjected to Solid-Solution Hardening

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Abstract—An approach is proposed to obtain regression relations to estimate the mechanical properties of steels subjected to solid-solution hardening. The applicability of the developed approach is shown for hot-rolled sheet austenitic iron–nickel and nickel alloys after quenching, toughened low-alloy structural steels with a sorbite structure in the case of full hardenabilty, sheet corrosion-resistant ferritic steels after softening heat treatment, and corrosion-resistant austenitic steels after austenitization. The derived regression relations serve as the basis for correcting the chemical composition of a metal melt to ensure the required level of the mechanical properties of ready products by controlling the degree of solid-solution hardening.

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INTRODUCTION

The alloying elements in steels and alloys influence the physicochemical phenomena that accompany heat treatment, thermomechanical treatment, chemicothermal treatment, hot and cold metal forming, casting, and welding. In combination with other factors and parameters of action of a metal, they determine structure formation and the formation of mechanical properties in products.

The effect of various hardening mechanisms on the formation of yield strength σ_y in steels is reflected by the equation [1]

$$\sigma_y = \sigma_0 + \Delta\sigma_{ss} + \Delta\sigma_d + \Delta\sigma_{ph} + \Delta\sigma_{gb}, \quad (1)$$

where $\Delta\sigma_{ss}$, $\Delta\sigma_d$, $\Delta\sigma_{ph}$, and $\Delta\sigma_{gb}$ are the contributions of the solid-solution hardening, dislocation hardening, precipitation hardening, and grain-boundary hardening, respectively, and σ_0 is the friction stress of the iron lattice.

As a rule, commercial products meet the condition

$$A = \sigma_0 + \Delta\sigma_d + \Delta\sigma_{ph} + \Delta\sigma_{gb} \approx \text{const}. \quad (2)$$

Then, Eq. (1) can be rewritten as

$$\sigma_y = A + \Delta\sigma_{ss}. \quad (3)$$

Solid-solution hardening is achieved for a set of various physical phenomena. Alloying elements create elastic strain fields in a crystal lattice, which retard dislocations, change the stacking-fault energy, change the Peierls–Nabarro force, and increases the friction force during the motion of an edge dislocation by hindering its cross sliding when it bypasses a dissolved atom. Dislocation motion is retarded by the electric interaction of dislocations and the ions of the elements that form a solid solution along with the ordering-induced appearance of obstacles to dislocations during the complication of an intragranular structure and the formation of surface defects in the form of antiphase boundaries and domain walls. Impurity atoms form Cottrell, Snoek, and Suzuki atmospheres and, hence, block dislocations. The interaction of the elements dissolved in the crystal lattice of a matrix also influences the degree of strain hardening [2].

The degree of solid-solution hardening can be quantitatively described using the Mott–Nabarro theory, according to which the local internal stresses caused by dissolved atoms mainly depend on the difference between the atomic radii of a dissolved element and the solvent. The solid-solution hardening is proportional to the atomic size misfit of a dissolved component and the alloy matrix [2],

$$\delta_r = (r_{de} - r_m)/r_m. \quad (4)$$

The atomic radius is determined as half the interatomic distance and depends on the state of atomic bonding [3]. Therefore, the characteristics of atomic bonding, including the degrees of metallicity (C_m) and covalence (C_c) functionally determine δ_r. Thus, a relation between C_m and C_c, on the one hand, and the solid-solution hardening of steels, on the other, should exist according to the Mott–Nabarro theory. The purpose of this work is to find this relation, which determines (according to Eq. (3)) the influence of dissolved atoms on the mechanical properties of the metal of end product.

EXPERIMENTAL TECHNIQUE AND RESULTS

In steels and alloys the characteristics of metallicity and covalence of all interatomic bonds of matrix atoms and the bonds of matrix atoms with alloying elements and impurities are the generalized degrees of metallicity (C_m^{gen}) and covalence (C_c^{gen}). These characteristics are determined by the formulas [4]

$$C_c^{gen} = \sum_{i=1}^{N} C_{ci}X_i, \quad C_m^{gen} = \sum_{i=i}^{N} C_{mi}X_i, \tag{5}$$

where C_{ci} and C_{mi} are the degrees of covalence and metallicity, respectively, that characterize the ith ($i = 1, \ldots, N$) interatomic bond and X_i is the mole fraction of the dissolved atom participating in the formation of the ith chemical bond.

By analogy with Eq. (5), we introduce the generalized degree of metallicity of all interatomic bonds in a substitutional solid solution (C_m^{sss}) and the degree of covalence C_c^{iss}, which characterizes all interatomic bonds in an interstitial solid solution,

$$C_m^{sss} = \sum_{j=1}^{K} C_{mj}X_j, \tag{6}$$

$$C_c^{iss} = \sum_{i=1}^{M} C_{ci}X_i. \tag{7}$$

Here, j ($j = 1, \ldots, K$) is the index of chemical bond in the substitutional solid solution, C_{mj} is the metallicity of the jth interatomic bond, X_j is the mole fraction of element atoms in the substitutional solid solution calculated without regard for interstitial atoms in the chemical composition of steel or alloy, l ($l = 1, \ldots, M$) is the index of chemical bond in the interstitial solid solution, C_{cl} is the covalence of the lth interatomic bond, and X_l is the mole fraction of element atoms in the interstitial solid solution calculated without regard for substitutional atoms in the matrix composition. C_{cl} and C_{mj} of the possible interatomic bonds in steels and alloys were calculated by the technique from [5] for the electronegativities of elements from [6, 7] with allowance for the coordination numbers of substitutional and interstitial atoms and the stoichiometric coefficients of chemical compounds.

When correlation relations are constructed for solid-solution hardening, the hardening contribution of dissolved atoms is usually taken into account in terms of their mass concentrations and hardening factors [8]. For example, for the yield strength of alloyed ferrite, we have

$$\sigma_y = A_0 + \sum_i k_i^{el}[E_i], \tag{8}$$

where A_0 is the parameter that takes into account the contributions of all types of hardening except for solid-solution hardening to σ_y, i is the index of the dissolved element, k_i^{el} is the hardening factor, and $[E_i]$ is the mass concentration of dissolved element atoms.

The type of chemical element and its concentration influence the state of interatomic bonds and, correspondingly, parameter δ_r (see Eq. (4)) in the Mott–Nabarro theory. However, correlation relation (8) does not take into account the effects of the joint effect of dissolved atoms of different types. This disadvantage can be avoided if we use independent variables in the form of the direct characteristics of the state of interatomic bonds (C_m^{sss}, C_c^{iss}), which are functions of the contents of all dissolved atoms in substitutional and interstitial solid solutions, instead of $[E_i]$.

The contribution to the hardening of a ferrite matrix of interstitial atoms and carbon, which forms an interstitial solid solution, has an additive character [8]. Nitrogen, which forms an interstitial solid solution in the austenite of corrosion-resistant steels, also additively increases the degree of solid-solution hardening [2]. This finding points to a general law, which consists in an additive character of influence of interstitial and substitutional solid solutions on the solid-solution hardening of alloyed ferrite and austenite.

It follows from the aforesaid that, when condition (2) is met, the correlation relationship for estimating the yield strength of steels caused by solid-solution hardening can be written as

$$\sigma_y = a_{\sigma_y} + b_{\sigma_y}C_m^{sss} + d_{\sigma_y}C_c^{iss}, \tag{9}$$

where a_{σ_y}, b_{σ_y}, and d_{σ_y} are the coefficients determined by regression analysis.

By analogy with Eq. (9), we can present correlation relationships for estimating other mechanical properties of steels to a first approximation in the form

$$\sigma_u = a_{\sigma_u} + b_{\sigma_u}C_m^{sss} + d_{\sigma_u}C_c^{iss}, \tag{10}$$

$$\delta = a_\delta + b_\delta C_m^{sss} + d_\delta C_c^{iss}, \tag{11}$$

$$\psi = a_\psi + b_\psi C_m^{sss} - d_\psi C_c^{iss}, \tag{12}$$

where σ_u is the ultimate tensile strength; δ is the relative elongation; ψ is the relative reduction of area; and a_{σ_u}, a_δ, a_ψ, b_{σ_u}, b_δ, b_ψ, d_{σ_u}, d_δ, and d_ψ are the coefficients determined by regression analysis.

Austenitic Steels

We analyzed the mechanical properties of the following corrosion-resistant austenitic steels [9]: 10Kh14G14N4T, 09Kh14N19V2BR, 08Kh16N13M2B, 12Kh17G9AN4, 10Kh17N13M2T, 10Kh17N13M3T, 12Kh18N9, 12Kh18N9T, 04Kh18N10, 08Kh18N10,

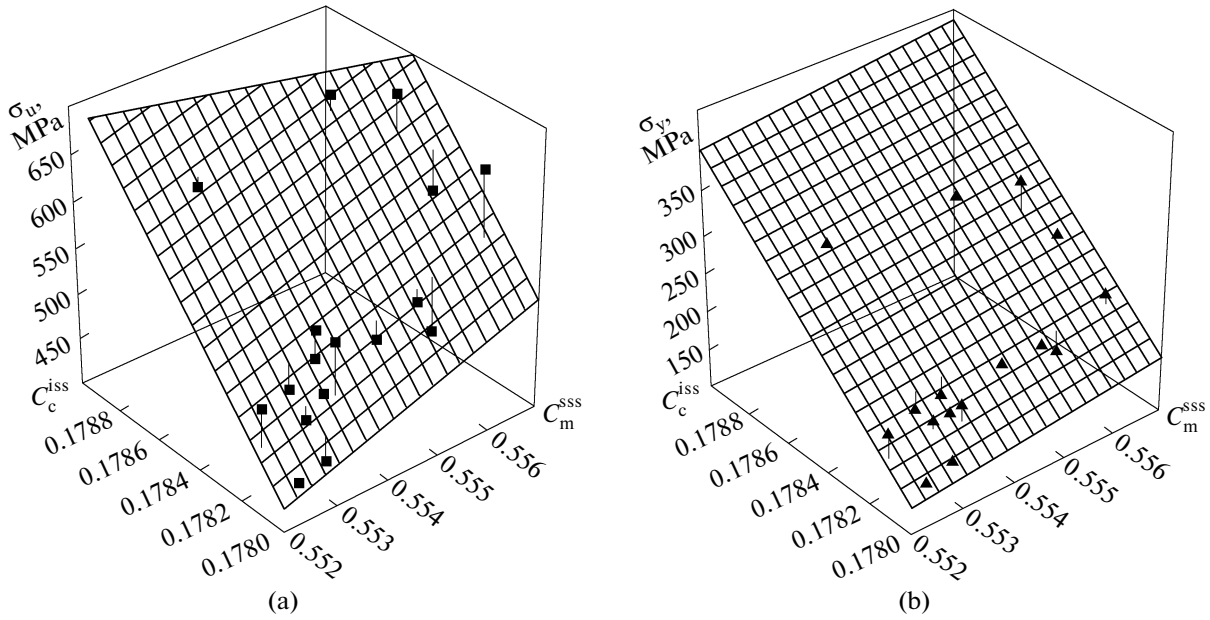

Fig. 1. (points) Experimental data in the regression planes described by Eq. (13) for (a) ultimate tensile strength ($R = 0.89$) and by Eq. (14) for (b) conventional yield strength ($R = 0.95$) of some corrosion-resistant austenitic steels.

08Kh18N10T, 12Kh18N10T, 03Kh18N11, 36Kh18N25S2, 07Kh21G7AN5, 10Kh23N18, and 20Kh25N20S2. These steels were subjected to austenitization and had chemical compositions according to [10] for the case of the minimum content of substitutional atoms and the maximum content of atoms of other elements.

The ultimate tensile strength and the yield strength of these steels are approximated by the following regression equations, which were derived by multiple regression analysis using Eqs. (9) and (10) [9]:

$$\sigma_u = -64276.6 + 18608.29C_m^{sss} + 305789.9C_c^{iss}, \quad (13)$$

$$\sigma_y = -58931 + 8112.245C_m^{sss} + 306690C_c^{iss}. \quad (14)$$

Figure 1 shows the experimental data from [9], the regression planes for Eqs. (13) and (14), coefficients of correlation R.

Toughened Structural Steels

In the case of incomplete hardenability upon quenching, toughened structural steels form other products of austenite decomposition (upper and lower bainite, ferrite–pearlite mixture) along with martensite, which strongly influences their mechanical properties [8]. Using this fact and requirement (2), we analyzed a set of hot-rolled low-alloy structural steels subjected to quenching followed by high tempering to form sorbite at the wall thickness that ensured full hardenability in order to test the applicability of Eqs. (9)–(12). The chemical compositions and the mechanical properties of the set included the following steels [11]: 18KhGT, 20Kh, 30G, 40G, 20KhR, 45KhTs, 45Kh, 09G2, 35G2, 38KhS, 40KhFA, 30KhN3A, 35Kh2GSVA, 40KhFMA, 38Kh2N2MA, 15Kh2GN2TRA, and 38KhMYuA.

For the set of mechanical properties and the values of C_m^{sss} and C_c^{iss} calculated by Eqs. (6) and (7) for these steels, correlation relationships (user-defined functions) (9)–(12) are transformed into the following regression equations using multiple regression analysis:

$$\sigma_u = -208230.857 + 276675.186C_m^{sss} + 304049.58C_c^{iss}, \quad (15)$$

$$\sigma_{0.2} = -202856 + 261429.1C_m^{sss} + 319204.9311C_c^{iss}, \quad (16)$$

$$\delta = 3447.902 - 4399.38C_m^{sss} - 5386.08C_c^{iss}, \quad (17)$$

$$\psi = 6744.468 - 6256.74C_m^{sss} - 17178.3C_c^{iss}. \quad (18)$$

Figure 2 shows the experimental mechanical properties of the toughened structural steels and the approximating planes of multiple regressions (15)–(18) [11].

Austenitic Iron–Nickel and Nickel Alloys

Using multiple regression analysis and correlation relationship (10), we obtained the equation

$$\sigma_u = -398229 + 64111.75C_m^{sss} + 2039001C_c^{iss} \quad (19)$$

for the ultimate tensile strength of rolled sheets made of iron–nickel alloys KhN32T, KhN38VT,

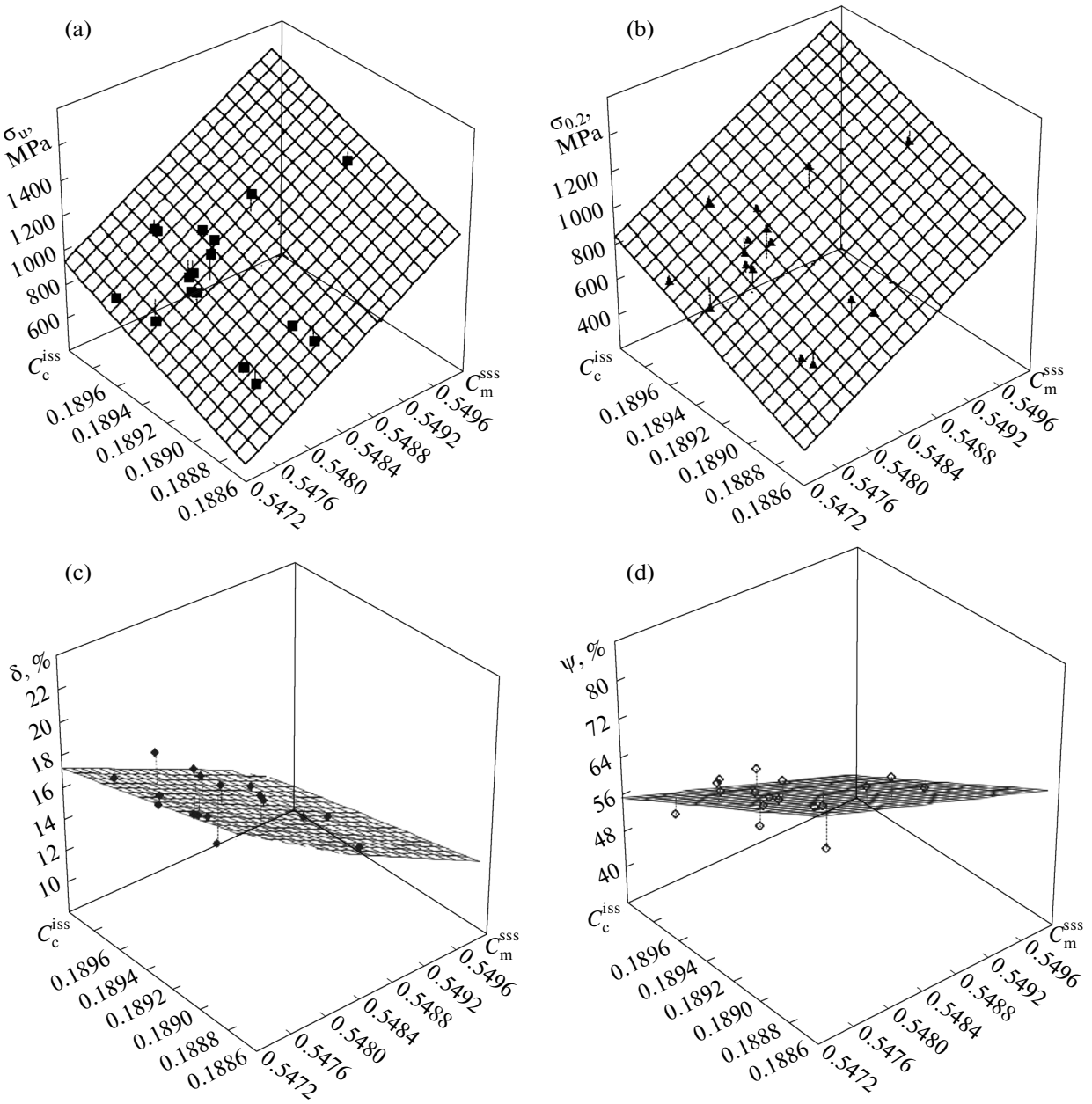

Fig. 2. (points) Experimental data in the regression planes described by the equations for (a) ultimate tensile strength ($R = 0.89$), (b) conventional yield strength ($R = 0.89$), (c) relative elongation ($R = 0.92$), and (d) relative reduction of area ($R = 0.84$) some toughened structural steels.

Kh28VMAB, and KhN45Yu and nickel alloys KhN70Yu, Kh75MBTYu, KhN58V, KhN65MV, and KhN78T after quenching [12] with the chemical compositions according to [10] (at the maximum content of alloying elements and impurities).

Figure 3 shows the ultimate tensile strengths of the alloys [12] and the regression plane calculated by Eq. (19).

Ferritic Steels

We analyzed the following sheet corrosion-resistant ferritic steels after softening heat treatment [13]: 08Kh13, 12Kh17, 08Kh17T, 15Kh25T, 15Kh28, 08Kh18T1, and 08Kh18Tch. The chemical compositions correspond to [10] for the case of the minimum content of substitutional atoms and the maximum content of atoms of other elements. To estimate the ultimate tensile strengths of these steels, we used the regression equation

$$\sigma_u = -39522.2 + 9245.608C_m^{sss} + 184601C_c^{iss}, \quad (20)$$

which was deduced by multiple regression analysis using correlation relationship (10).

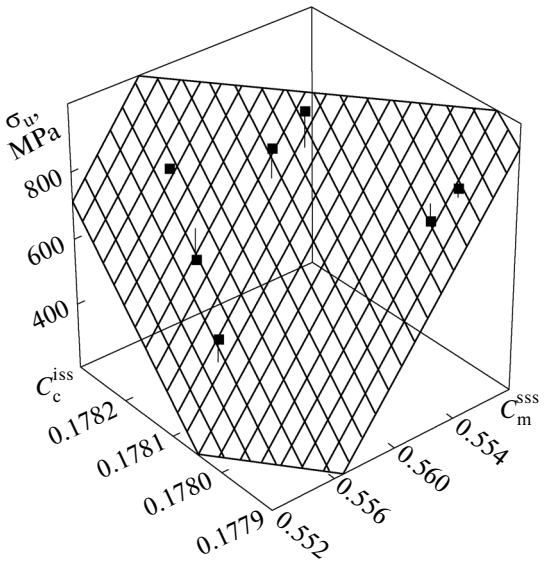

Fig. 3. (points) Experimental data in the regression planes described by Eq. (19) for the ultimate tensile strength (R = 0.91) of some iron–nickel and nickel alloys.

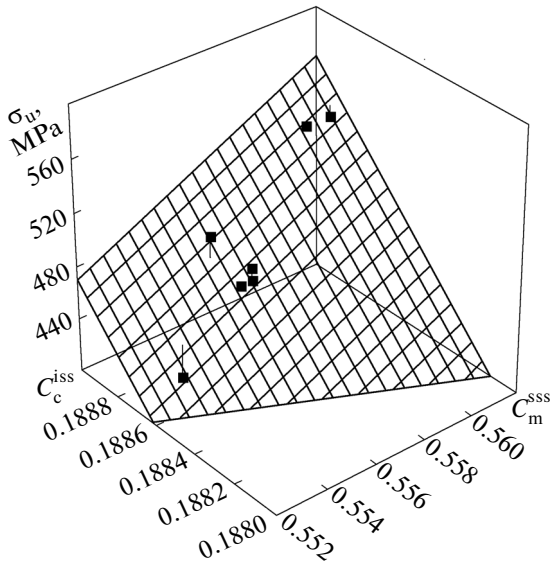

Fig. 4. (points) Experimental data in the regression planes described by Eq. (20) for the ultimate tensile strength (R = 0.952) of sheet corrosion-resistant ferritic steels.

Figure 4 shows the ultimate tensile strengths of these steels given in [13] and the regression plane calculated by Eq. (20).

DISCUSSION

The coefficients of correlation during the approximation of the experimental data by regression equations (13)–(20) exceed the critical values of the Pearson coefficient for the set under study at a significance level of 0.01 for the alloys and 0.001 for the steels. This finding indicates the presence of a linear relation between the degrees of metallicity and covalence (C_m^{sss}, C_c^{iss}) and the mechanical properties of the steels and alloys and supports the applicability of correlation relationships (9)–(12) for practice.

From Eqs. (14) and (16), we cannot separate the absolute contributions of substitutional and interstitial solid solutions to the mechanical properties of steel. Nevertheless, we can compare them with each other. To this end, we rewrite Eqs. (11)–(14) to separate solid-solution hardening factors $H_{\sigma_y}^A$ and $H_{\sigma_{0.2}}^S$. As a result, we obtain

$$\begin{cases} \sigma_y = -58931 + 8112.245 H_{\sigma_y}^A, & (21) \\ H_{\sigma_y}^A = C_m^{sss} + 38.806 C_c^{iss}, & (22) \end{cases}$$

for corrosion-resistant austenitic steels;

$$\begin{cases} \sigma_{0.2} = -202856 + 261429.1 H_{\sigma_{0.2}}^S, & (23) \\ H_{\sigma_{0.2}}^S = C_m^{sss} + 1.221 C_c^{iss}. & (24) \end{cases}$$

for toughened structural steels.

The coefficients before C_c^{iss} in hardening factors $H_{\sigma_y}^A$ and $H_{\sigma_{0.2}}^{S.}$ can be used to estimate the effect of an interstitial solid solution on the mechanical properties of the steels to be compared. These coefficients in Eqs. (21)–(24) indicate that the interstitial solid solution exerts a much stronger hardening effect in corrosion-resistant austenitic steels than in toughened structural steels.

Carbides and nitrides begin to form in nitrogen-bearing austenitic steels with C + N_2 > 0.3 wt % [13]. The formation of Fe_2N is accompanied by a decrease in the number of Fe–Fe bonds in a substitutional solid solution and, correspondingly, an increase in the contribution of Fe–Cr and Fe–Mn bonds, which are more metallic than Fe–Fe bonds, to C_c^{iss}. The appearance of Fe_2N also increases C_c^{iss}; according to Eqs. (13) and (14), this also causes an increase in the strength properties. In the case of formation of iron carbides, carbon also favors an increase in C_m^{sss} and C_c^{iss} but to a lesser extent than nitrogen.

Thus, carbon or nitrogen alloying of austenitic steels enhances the metallic character of interatomic bonds in a substitutional solid solution, which eventually results in hardening. This hardening mechanism was experimentally supported in [13].

For the yield strength of toughened structural steels, parameter $A_{exp} = \Delta\sigma_1/\Delta\sigma_2$, where $\Delta\sigma_1$ and $\Delta\sigma_2$ are the hardening contributions of substitutional and interstitial solid solutions, respectively, can be esti-

mated by the quantity $A_{calc} \approx C_m^{sss}/1.221C_c^{iss}$ using the physical meaning of Eq. (24).

For example, for the 15KhN5MF steel with the chemical composition from [14], we have $C_m^{sss} = 0.54896$ and $C_c^{iss} = 0.18882$ and $\sigma_{0.2} = 931 \pm 180$ MPa, according to Eq. (16). This calculated value is close to the experimental value for this steel (1130 MPa) after quenching and medium tempering at 400°C to form sorbite [14]. This fact means that condition (2) for the set of toughened low-alloy steel under study is approximately fulfilled for the 15KhN5MF steel in this structural state; that is, its experimental mechanical properties can be used in comparative calculations.

For the structural state of the 15KhN5MF steel under study, we have $\Delta\sigma_1 = 33.3$ and $\Delta\sigma_2 = 14.7$ MPa and, correspondingly, $A_{exp} = 2.27$ [14]. The calculated value ($A_{calc} = 2.38$) differs from A_{exp} by 5%. Good agreement between parameters A_{exp} and A_{calc} indicates that the terms of hardening factor $H_{\sigma_{0.2}}^S$ in Eq. (24) can be applied to compare the hardening contributions of the substitutional and interstitial solid solutions in the toughened low-alloy structural steels under study.

When deriving regression equations (13)–(20) by multiple regression analysis in correlation relationships (9)–(12), which are user-defined functions, we used independent variables in the form of generalized characteristics of interatomic bonds in a substitutional solid solution (C_m^{sss}) and an interstitial solid solution (C_c^{iss}). According to Eqs. (6) and (7), these characteristics also depend on the chemical composition of an alloy or steel. The required values of C_m^{sss} and C_c^{iss} that determine the required mechanical properties in Eqs. (13)–(20) can be reached for many combinations of various types of dissolved atoms at various concentrations. As a result, the obtained regression equations can be used to control the degree of solid-solution hardening via the optimization of the chemical composition of steel and alloy.

CONCLUSIONS

(1) We derived correlation equations (9)–(12) to obtain regression equations to estimate the mechanical properties of steels. As examples, we considered sets of hot-rolled sheet austenitic iron–nickel and nickel alloys after quenching, toughened low-alloy structural steels with a sorbite structure in the case of full hardenabilty, sheet corrosion-resistant ferritic steels after softening heat treatment, and corrosion-resistant austenitic steels after austenitization.

(2) According to Eqs. (6) and (7), independent variables C_m^{sss} and C_c^{iss} in Eqs. (9)–(12) can have the same values at various versions of content of alloying elements and impurities. As a result, the required mechanical properties of products can be achieved by changing the concentrations of impurities and alloying elements within the ranges of specified chemical compositions of steel and alloys grades. Since condition (2) determines the applicability of Eqs. (9)–(12) for ready products, the regression equations derived from them can be used to correct the chemical composition of steel at the stage of melting or forming a welded joint in order to ensure the required and stable level of the mechanical properties of products by controlling the degree of solid-solution hardening.

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