ГАЛУЗЕВЕ МАШИНОБУДУВАННЯ

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OPTIMIZATION OF THE CHEMICAL COMPOSITION OF STEEL FOR ENGINEERING STRUCTURES BY THE CRITERION OF STABILIZATION OF MECHANICAL PROPERTIES

Summary. The aim of the study is to create a mathematical model for the operational control of the strength characteristics of the expected metal structure in the conditions of serial steelmaking. Traditional approaches based on test results of prototypes obtained in laboratory conditions are not suitable for this purpose. This is because, in mass production steelmaking, the strength characteristics of products are affected by the metal structure and many other melting conditions, in addition to their chemical composition. This justifies the need to take into account the parameters of interatomic interaction as optimization criteria.

The main idea of the study is to take into account the concept of directional chemical bonding of metal, which links their composition, structure and metal properties.

This concept is supplemented by elements of optimization of the chemical composition of steel, by the criterion of stabilization of mechanical properties, and by methods of planning experiments. This allowed us to obtain variation intervals for the main optimization criteria.

To ensure the physical essence of the models for predicting the mechanical properties of steels of railway equipment bearing systems, it is proposed to use integral physical and chemical criteria: the structural parameter d (nm 10-1) and the physical and chemical equivalent $Z_Y(e)$.

The influence of alloying elements (chromium, molybdenum, vanadium) on the formation of mechanical properties of steel is studied on the basis of mathematical and physicochemical modelling. The intervals of alloying elements content that ensure compliance with the required standards are determined. Dependencies of changes in the mechanical properties of alloyed rolled products on the structural state index d were constructed.

The intersection of the functions of properties of medium-carbon steels in the eutectic region corresponds to the provisions of N.S Kurnakova aw, and makes it possible to predict the level and combination of properties and characteristics of alloys.

Keywords: mathematical functions, tensile strength, freight transportation, carbon, relative elongation, mathematical models, factor analysis, chemical composition of steel, reliability, mechanics, computer modelling, automation.

Problem statement. Modern mechanical engineering imposes increasingly high requirements to the operational properties of materials [1]. By applying various technological schemes of heat treatment of alloyed rolled products, it is possible to change the strength properties by influencing the processes of structure formation. Mechanical and operational properties of metal are determined by the structure of metal, which depends on the chemical composition, deformation conditions, temperature and cooling mode. It is known that the content of chemical elements in the steel composition has a decisive influence on structure formation during heat treatment. Attempts to experimentally investigate the dependences of mechanical properties of steels on their chemical composition and the construction of mathematical models based on the results of experiments have been going on for decades.

Analyses of the latest research and publications. Ohkubo N. et al. back in 1994 published an article [2] reporting on a series of experiments with prototype samples of austenitic stainless steel with different chemical compositions including carbon, silicon, manganese, phosphorus, sulfur, nickel, chromium, molybdenum, copper, nitrogen. As a result of these experiments, the authors obtained experimental curves of hardness, yield strength and tensile strength as a function of grain size and percentage of the above chemical elements. The experimental curves were then approximated by linear regression equations, which were then used to analyze the results obtained.

Han et al. [3], using the example of hot-rolled ribbed bar production, obtained linear regression equations expressing the dependence of strength, yield strength and relative elongation on the content of carbon, manganese, chromium, nickel, vanadium. With the help of mathematical model they obtained an acceptable range of chromium content, which does not reduce the quality of manufactured products, which provides, in their opinion, the most favorable in operational terms mechanical properties of prototypes.

Sheyko et al. [4] performed the following series of laboratory experiments. Laboratory castings with different content of alloying elements were produced in an induction furnace and then forged into 10×80×120 mm billets, whose mechanical characteristics were determined: tensile strength, yield strength, relative elongation, and impact toughness. Having processed the experimental results, the authors [4] obtained regression equations reflecting the dependence of mechanical properties of the tested low-carbon steel on the content of alloying elements: chromium, titanium and vanadium. With the help of these dependencies, they selected the optimal combinations of alloying elements, providing, in their opinion, the most favorable in operational terms mechanical properties of test specimens.

However, V.A. Lutsenko et al. [5] criticized such approaches. They noted that ‘existing approaches to the optimization of the chemical composition of steel, providing the necessary mechanical properties of steel products, are usually based on statistical models of composition – property roller and do not reflect the physical and chemical aspects of the behavior of multi-component melt at the final stages of the technology of obtaining finished products. In this regard, the authors [5] advise to use the following approach. Since phase transformations are a consequence of interatomic interactions in a multicomponent melt, it is suggested to use the dance pattern of the chemical composition through the structural state parameter d. In physical terms, the parameter d represents the average inter-nuclear distance between interacting atoms of the investigated steel. Using this approach, the authors [5] studied the influence of alloying elements (chromium, molybdvanadium) on the formation of mechanical properties of steel. They plotted the dependences of tensile strength and relative elongation on the physicochemical criterion – structural modelling parameter d. As a result, it is shown that the increase in chromium content increases the tensile strength, and alloying with molybdenum and vanadium increases ductility.

In metallurgy there is a fundamental law linking the properties of alloys with their composition and structural state – the law of N.S. Kurnakov [6]. One of the basic provisions of this law is the absence of function discontinuity within one phase region of the state diagram. Thus, the development of

new and optimization of existing compositions of structural steels by reducing the carbon content by compensating it as a hardener by elements of matrix micro alloying systems (C, Si, Mn,) is an urgent task [7–9].

Formulation of the objectives of the article. Improvement of mechanical, exploitation characteristics, and physical and chemical properties of steels of machine-building structures due to optimization of the chemical composition of steel for the criterion of stabilization of mechanical properties.

Teaching the core material. Steels, as structural materials, have great opportunities to increase their quality and improve all service properties by improving their production technology, reducing harmful impurities, alloying and microalloying, taking into account the physical and chemical nature and physical structure of the materials. Structural steels are usually subject to the following requirements: a combination of high structural strength and sufficient toughness.

In automobile, shipbuilding, railway engineering are widely used critical parts that must have wear resistance and strength under conditions of high pressures, loads and temperatures (nozzles, sleeves, plunger pairs, wheel pairs, bearing elements, etc.) Increasing the load capacity to the axial load of freight cars can be achieved by increasing the axial load up to 25 tonnes, the use of new design solutions, as well as through the use of new structural materials with increased strength.

One of the brightest representatives of such steels is 09G2S steel. The advantage of this steel is that it is not prone to tempering brittleness, which in turn allows for a wide range of tempering temperatures. To date, the most widely used for the load-bearing structures of cars is low-alloy steel grade 09G2S according to DSTU 8541:2015 Rolled steel of increased strength. Technical conditions [10].

The greatest application has rolled steel of strength class 325 (kingpin beam, individual elements of the car with a thickness of 10 mm and more) and 345 (individual elements of the car with a thickness of less than 10 mm). At the same time, steels with higher mechanical properties are widely used in other branches of heavy machine building. For example, high-strength steels with yield strength of 400 MPa and more are used for manufacturing and repair of mining equipment, quarry machinery and attachments, power structures of lifting mechanisms and cargo vehicles [11]. There are known cases of application of steels with yield strength of 550 MPa and more in wagon building [1].

In order to assess the influence of the chemical composition of steel on its mechanical properties and temperatures of phase transformations, the concept of directed chemical bonding in the description of interatomic interaction in the melt developed in the Institute of Chemistry of NASU [12,13] was used. The principle of this concept is to describe the chemical composition of the melt by a complex of integral model parameters of interatomic interaction. It allows to reduce the parametricity of models in which the element-by-element composition of multicomponent steels T is expressed in integral parameters of interatomic interaction.

Preliminary, the factor analysis by the method of head components has been carried out. The measure of informativity of the factors is the ratio of dispersions of head components and input data [14]. On the basis of which the structuring of the chemistry of steel into various subsystems was performed, the most significant of which were:

a) matrix m (C, Si, Mn)

b) light subsystem ml includes (Cr, Ni, Gu)

c) domic acid subsystem includes domic acid (S), phosphorus (P)

(Fig. 1) shows the results of structuration of the chemical composition of structural steel O9G2S behind the load on the main integral factors. On the basis of factor analysis, integral parameters for matrix and impurity subsystems were calculated. (Fig.1) shows the dependences between mechanical properties and parameters of interatomic interaction of impurity subsystems. From the given dependences, it follows that, a significant contribution to the formation of the relative elongation is made by the impurity subsystem (Cr, Ni, Gu), and for the strength limit – by the matrix subsystem (C, Si, Mn).

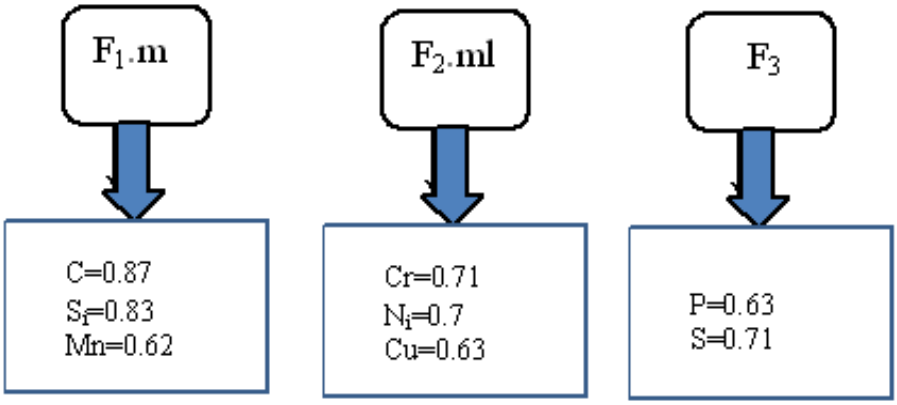

Fig. 1. Significant loadings on integral factors

Solution of the problem of dimensionality reduction of prediction problems based on the theory of directed chemical bonding [15]. Since phase transformations are a consequence of interatomic interaction in a multicomponent melt, at the first stage the chemical composition is 'reconciled' through the integral parameters of charge $Z^Y(e)$ and structural d (nm 10^{-1}) state, which are calculated as a result of pairwise interaction of all its m components by solving the system of nonlinear m^2-m+1 equations:[12].

$$\begin{cases} a - f(\Delta e'_{ij}) = 0, \\ a - f(\Delta e''_{ij}) = 0, \qquad i = 1,2,...,m-1, j = i+1,...,m, \\ 4 \cdot Z^X(a, \Delta e') + Z^Y(d, \Delta e'') = 0, \end{cases} \tag{1}$$

where $\Delta' e_{ij}$ – the number of electrons that are localized by the interaction in the direction of bond i-j at distance a (on the diagonal of the OCC or HCC lattices);

$\Delta'' e_{ij}$ – at a distance d=0.866*a· along the face:

$$\begin{aligned} \Delta e' &= (\Delta e'_{12}, \Delta e'_{13}, .\Delta e'_{ij}., \Delta e'_{m-1,m}), \\ \Delta e'' &= (\Delta e''_{12}, \Delta e''_{13}, .\Delta e''_{ij}., \Delta e''_{m-1,m}) \end{aligned} \tag{2}$$

As a result of solving the above nonlinear system of equations, the following are determined:

$$a, \Delta e'_{ij}, \Delta e''_{ij}, i = 1,...,m-1, j = i+1,...,m. \tag{3}$$

The parameter Z^Y is determined by averaging the effective charges of all i –j bond types with bond length d:

$$Z^Y = \sum_{k=1}^{m} \frac{\lg Ru_k^o - \lg(d/2)}{tg\alpha_k} \cdot n_k^2 + 2 \cdot \sum_{k=1}^{m-1} \sum_{l=k+1}^{m} n_k \cdot n_l \cdot \Delta e''_{kl}, \tag{4}$$

where n_k – mole fraction, Ru^0_k – is the radius of the unpolarised atom,

$tg\alpha_k$ – parameter, which characterises the change of electron density at ionisation of the atom of the k-th component.

tgα – gradient of change of the ion radius at change of its charge

In the above formulation, the purpose of optimising the chemical composition of the study of steels in engineering structures by optimising the chemical composition of steel according to the criterion of stabilising mechanical properties can be considered as a multidimensional optimisation problem

with constraints [17] is to determine the corresponding vector of controlled parameters in the domain D $\overline{X}^*(x_1^*, x_2^*, ...x_k^*)$, the values of which ensure the achievement of an extreme value of the objective function $y_{gen} = F(\overline{X}^*)$ and satisfy all the given functional constraints that define the domain $Д_X$.

Then the mathematical formulation of the optimisation problem can be represented as follows:

$$y_{gen} = F(\overline{X}^*) = extremum \tag{5}$$

$$\overline{X}^* \in Д_X \in Д .$$

In this case, the domain of possible solutions, determined by the intervals of variation of the variable parameters $x_1, x_2, ..., x_k$

$$Д = \left\{ \overline{X} \Big|_{x_{i\min} \le x_i \le x_{i\max};\, i \in [1;n]} \right\} \tag{6}$$

The domain of acceptable solutions, taking into account factor constraints $y_l \le a$, ..., $y_j = b$

$$Д_x = \left\{ \overline{X} \Big|_{y_l \le a, ..., y_j = b; x_{i\min} \le x_i \le x_{i\max};\, i \in [1;k]} \right\} \tag{7}$$

The analysis of numerous scientific studies in the direction of analysing the influence of the chemical composition of steel on the mechanical properties of steel [2–8; 11–16] made it possible to identify the following groups of requirements (structural components of the Y vector) that should be taken into account when optimising the chemical composition.

Group 1. Physicochemical Criterion. Interatomic interaction d. and integral parameters of charge Z^Y, as a "convolution" of chemical composition as well as structural parameter d (nm 10^{-1}) d. component gradient of change of ion radius with change of its charge,tgα, cooling rate V_{ohl},;

Group 2. Criterion factorisation matrix m (C, Si, Mn);

Group 3. Criterion of mechanical properties: such as tensile strength (σv), yield strength (σ_T), elongation (δ);

In (Fig. 2–3) as an application is presented additional graphs to the identification of optimal parameters of steel for the criterion of stabilisation.

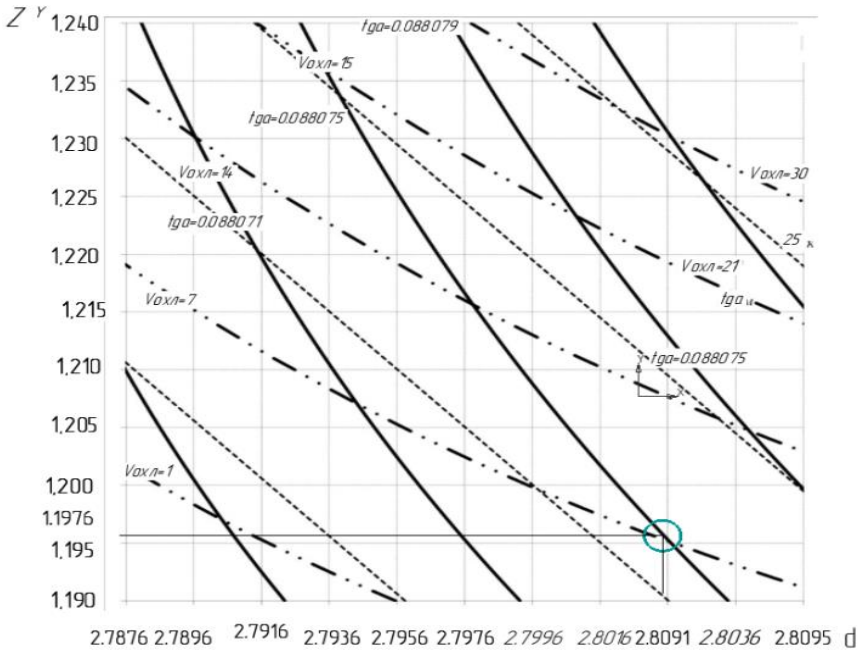

Fig. 2. Structure-charge diagram optimisations for physico-chemical criteria

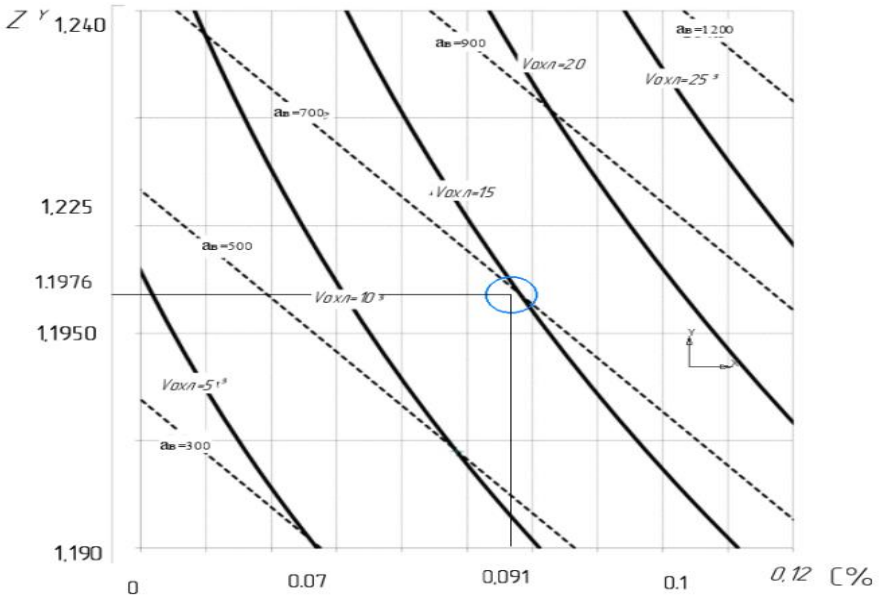

Fig. 3. Dependence of the Z^Y parameter the charge state of the system

(Tables 1 and 2) summarise the optimal steel parameters obtained for the criterion of mechanical property stabilisation and their comparison with DSTU and commercial samples.

Table 1

Actual and optimised chemical composition of 09G2S steel, wt%

Riznovid Khimichny warehouse	Mass fraction of elements % wt.							
	C	Si	Mn	Cr	Ni	Cu	P	S
Promislovies[19]	0,10	0,6	1,5	0,03	0,03	0,3	0,025	0,03
Optimal	**≤0,091**	**≤0,23**	**≤1,71**	**≤0,027**	**≤0,027**	**≤0,201**	**≤0,009**	**≤0,007**
DSTU 8541:2015	≤0,12	0,17-0,37	1,4-1,8	≤0,3	≤0,3	≤0,3	–	–

Table 2

Mechanical power of steel 09G2S, high chemical composition after normalization in industrial minds and optimization according to the criterion of stabilization of mechanical power

Mechanical power has become important as a criterion of brilliance						
	σ_v,МПа	Q(σ_v)	$\underline{\sigma_T}$ МПа	Q(σт)	δ %	Q(δ)
Promislovies	490 (4)	0,95	345 (6)	0,98	21	–
Optimal	**750 (56)**	**0,95**	**570 (65)**	**0,98**	**21**	**–**
DSTU 8541:2015	≥480	–	≥345		≥21	–
In brackets () is the standard deviation						

Conclusions.

1. The kink of the functions of properties of medium-carbon steels in the eutectic region corresponds to the provisions of N.S. Kurnakov law and allows predicting the level and combination of properties and characteristics of alloys.

2. According to the results of the performed studies, it is shown that the optimisation of the chemical composition of the studied steels of engineering structures is possible due to the optimisation of the chemical composition of steel by the criterion of stabilisation of mechanical properties. The most significant parameters in the calculation of σ_v, σTare the integral parameters of interatomic interaction d, and Z^Y full matrix subsystem (C, Si, M_n), microalloying subsystem (C_r, N_i, G_u), and cooling rate V_{cool}.

3. The substantiated choice of the main elements of the chemical composition of 09G2S steel according to the criterion of stabilisation of mechanical properties, the main criterion and functional constraints, as well as the chosen technology for conducting an optimisation study, made it possible to search for such values. It was found that after the value of the charge state, when the condition $1.1960 \leq Z^Y \leq 1.2151$ is met, the trend lines of hardness values 'change' their position. Thus, it has been established that for low-alloy steels, the chemical composition of which has an optimised value of Z^Y=1.1971 or less, additional normalisation after hot plastic deformation is not effective in terms of increasing hardness. The optimised value of d = 2.8091 and the highest mechanical properties σ_v = 750 MPa, σ_T = 600 MPa, V_{oxl}.= 7 C/sec.

4. The obtained optimal chemical composition of 09G2S steel according to the criterion of stabilisation of mechanical properties does not contradict the information on the chemical compositions of structural steels obtained by a representative sample of industrial data with a wide variation in composition and properties reviewed in [19] and also meets the requirements of [10].

5. An analysis of the regulatory requirements for the content of the main chemical components of structural steels was carried out It was found that the standardised intervals are quite wide and largely overlap, which can cause a wide variation in the values of mechanical properties, provided that the steel meets the chemical composition requirements of the standard and is stable.

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Bibliography

1. Фомін О.В. Оптимізаційне проєктування елементів кузовів залізничних напіввагонів та організація їх виробництва : монографія. Донецьк : ДонІЗТ УкрДАЗТ, 2013. 251 с.

2. Ohkubo N., Miyakusu K., Uemats Y., Kimura H. Effect of alloying elements on the mechanical properties of the stable austenitic stainless steel. *ISIJ International.* 1994. Vol. 34. № 9. P. 764–772. https://doi.org/10.2355/isijinternational.34.764

3. Han R., Hu M., Pei Q., Gong D., Song Y. The influence of chemical element on properties of deformed steel bar. *Open Journal of Statistics.* 2016. Vol. 6. P. 1174–1180. http://dx.doi.org/10.4236/ojs.2016.66095

4. Sheyko S., Beloko Y., Kripak A., Shalomeev V., Tsyganov V., Kulabneva E. Development of rational chemical composition of special steel with increased mechanical and performance characteristics. *Journal of Chemical Technology and Metallurgy.* 2023. Vol. 58. № 4. P. 798–805. https://doi.org/10.59957/jctm.v58i4.114

5. Вплив хімічного складу на механічні властивості легованої сталі / В.А. Луценка та ін. *Лиття та металургія.* 2018. № 1 (90). С. 120–123.

6. Пахолюк А.П. Основи матеріалознавства і конструкційні матеріали : посібник. Львів : Світ, 2015. 172 с.

7. Prikhodko E., Petrov A. F. Physical−chemical criteria for description of the composition effect on salt melt structure and properties. *Functional Materials.* 2000. Vol. 7. № 1. P. 108–113.

8. Бурлуцький О.В., Фомін О.В., Ткаченко В.П. Формалізація структурно-речовинних перетворень в несучих системах вантажних вагонів у результаті термічних впливів у процесі зварювальних і правочних робіт. *Зб. наук. пр. Державного економіко-технологічного університету транспорту.* Київ, 2016. № 29. С. 54–71.

9. Gubskyi S.V., Yepifanov V., Chukhlib Y., Basova A., Okun M., Ivanova. Integrated approach to determine operational integrity of crane metal structure. *Periodica Polytechnica Mechanical Engineering.* 2022. Vol. 63. № 4. P. 319–325.

10. ДСТУ 8541:2015. Прокат сталевий підвищеної міцності. Технічні умови.

11. Нікітін В.М. Високоміцні сталі з економним легуванням для кар'єрного транспорту та гірничодобувної техніки. *Сталь.* 2016. № 10. С. 57–66.

12. Приходько Є.В. Ефективність комплексного легування сталі та сплавів. Київ : Наукова думка, 1995. 292 с.

13. Тогобицька Д.Н., Пиптюк В.П., Логозинський Ю.Н. Системний підхід до вибору оптимального елементного складу сталі, що забезпечує необхідний рівень механічних властивостей. *Системні технології : регіон. міжвуз. зб. наук. пр.* Дніпропетровськ, 2015. С. 91–97.

14. Пономаренко В.С., Гур'янова Л.С., Пельовий Я.Є. Актуальні проблеми системного аналізу та моделювання процесів управління : зб. наук. пр. Братислава–Харків : ВШЕМ – ХНЕУ ім. С. Кузнеця, 2023. 409 с.

15. Приходько Є.В., Тогобицька Д.М., Козачок О.С. Інформаційно-аналітична система стабілізації властивостей прокату. *Металознавство та обробка металів.* 2011. № 1. С. 39–43.

16. Погребна Н.Є., Куцова В.З., Котова Т.В. Механічна стабільність матеріалів : навч. посіб. Дніпро : НМетАУ, 2021. 109 с.

17. Єрмакова С.М. Математична теорія планування експерименту. М. : Наука, 1983. 392 с.

18. Математичне моделювання процесу термічної правки балки хребтової вантажних вагонів-платформ / О.В. Фомін та ін. *Вісник Східноукраїнського національного університету.* 2019. № 3 (251). С. 186–190.

19. Малинов Л.С., Бурова Д.В. Нетипова термообробка сталей 09H2S і EN36, в тому числі з витримкою в міжкритичному інтервалі температур (МКІТ). *Вісник Приазовського державного технічного університету. Сер. : Технічні науки.* 2013. Вип. 27. С. 73–82.

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ОПТИМІЗАЦІЯ ХІМІЧНОГО СКЛАДУ СТАЛІ МАШИНОБУДІВНИХ КОНСТРУКЦІЙ ЗА КРИТЕРІЄМ СТАБІЛІЗАЦІЇ МЕХАНІЧНИХ ВЛАСТИВОСТЕЙ

Анотація

Метою роботи є створення математичної моделі оперативного управління характеристиками міцності очікуваної металоконструкції в умовах серійного сталеплавильного виробництва. Традиційні підходи, що ґрунтуються на результатах випробувань дослідних зразків, одержуваних у лабораторних умовах, для цієї мети не підходять. Сказане пояснюється тим, що оскільки в умовах серійного сталеплавильного виробництва на характеристики міцності виробів, крім їх хімічного складу, впливає структура металу і безліч інших умов плавок, це обґрунтовує необхідність для врахування параметрів міжатомної взаємодії як критеріїв оптимізації.

Головна ідея дослідження полягає в тому, щоб під час прогнозування до уваги брали концепцію спрямованого хімічного зв'язку металу, що пов'язує між собою їх склад, структуру і властивості металу.

Представлена концепція доповнена елементами оптимізації хімічного складу сталі за критерієм стабілізації механічних властивостей, методами планування експериментів, завдяки чому було отримано інтервали варіювання основних критеріальних показників оптимізації.

Для забезпечення фізичної сутності моделей прогнозування механічних властивостей сталей несівних систем залізничної техніки запропоновано використовувати інтегральні фізико-хімічні критерії: структурний параметр d (нм 10^{-1}) і фізико-хімічний еквівалент $Z^{Y}(e)$.

На підставі математичного та фізико-хімічного моделювання вивчено вплив легуючих елементів (хром, молібден, ванадій) на формування механічних властивостей сталі. Визначено інтервали вмісту легувальних елементів, що забезпечують виконання необхідних норм. Побудовано залежності зміни механічних властивостей легованого прокату від показника структурного стану d.

Перетин функцій властивостей середньовуглецевих сталей у ділянці евтектоду відповідає положенням закону Н.С. Курнакова і дає змогу прогнозувати рівень і поєднання властивостей та характеристик сплавів.

Ключові слова: математична функція, межа міцності, вантажні перевезення, вуглець, відносне подовження, математичні моделі, факторний аналіз, хімічний склад сталі, надійність, механіка, комп'ютерне моделювання.