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Optimization of chemical composition of steel for railroad wheels providing stabilization of mechanical and increase of operational properties

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Abstract
In connection with the increase in axle loads of freight cars on the railways and the increase of their speed of movement, the requirements to the service and operational properties of railway wheels, including wear resistance and thermal resistance, are significantly increasing. One of the main factors affecting these indicators is the chemical composition of steel for railway wheels.
To determine the influence of chemical elements on the service properties of railway wheels, composition of steel was structured as a chemically unified system, which was carried out on the basis of factor and physic-chemical analyzes with separation of elements into subsystems: matrix, alloying, microalloying and impurity. In this method, the influence of each of the subsystems is considered comprehensively through the physic-chemical parameters of the "convolution" of the chemical composition of each of them, which reduces the parametric of the forecast models, increases their information capacity and allows obtaining adequate and stable models according to scheme "chemical composition - microstructure - mechanical properties of steels for railway wheels". On the basis of computational and laboratory experiments, the "restricted" limits and the proportions of the elemental composition are proved, which ensure the required mechanical properties and increase the resistance to thermal effects arising from the operation of railway wheels during braking were justified. The influence of vanadium as one of the effective micro-alloying elements, which have a positive effect on the strength properties of railway wheels has been established.
Keywords: RAILWAY WHEELS, CHEMICAL COMPOSITION, MECHANICAL PROPERTIES OF STEEL PRODUCTS, THERMODYNAMIC INFLUENCE, "NARROWED" RANGES, INTEGRAL PARAMETERS OF THE INTERATOMIC INTERACTION

The state of the question

When using the wheels in each of their elements, a complex rapidly changing in time system of compressive and tensile stresses occurs. Stresses in the wheel-rail contact lead to damage, the vast majority of which can be classified as tread surface wear, thermal defects, fatigue defects and brittle fracture of the metal. In addition, during braking in the contact zone of the wheel with the rail, rapid high-temperature heating of the rim metal above the critical temperature Ac_3 can occur followed by accelerated cooling, as a result of which phase recrystallization of the metal with the formation of a new structural component – martensite is possible in these areas. Structural transformations in local areas of the wheel rim cause internal stresses and, as a consequence, the emerging of microcracks, which under the action of impact loads and the emerging stress center at their apices develop into the rim and propagate along the boundary between the microvolume of the metal undergoing transformation and the base metal. This leads to formation of chips of thermal origin.

Therefore, strict requirements are imposed not only on the design of the wheel, but also on the quality of the material used to produce it. The wheel should have a high level of strength, plastic properties, impact toughness and fracture toughness with low sensitivity to thermal effects.

The necessary combination of properties is achieved mainly due to the selection of the optimal structural state of the metal, which is determined by the chemical composition of the wheel steel and the thermal treatment modes of the wheels. When choosing a material, we proceed from the specific operating conditions of the wheels and their purpose. Currently, the requirements for the wheel metal are significantly increased in connection with the planned increase in the railways of Ukraine of axle loads of freight cars up to 25 tons and a rise of the passenger trains speed. The problem of their wear and heat resistance is put first. Thus, the development of new composition and optimization of the existing one of wheel steels due to reducing the carbon content by compensating it as a reinforcing agent with elements of the matrix micro-alloying system (Si, Mn, V) is an urgent task.

The complexity of developing new steel grades for wheels is due to the necessity of meeting a number of special requirements. Above all wheel steel should have high wear resistance and contact strength. The easiest way to improve these characteristics is to increase the carbon content. However, to increase the resistance of wheel steel to the formation of a "white layer" on the rolling surface, which conduce the occurrence of defects of braking (thermal) origin, the carbon content in it must be reduced in order to reduce the tendency of the steel to thermal cracking and brittle failure. At the same time, the weakening of steel become necessary to compensate by the introduction of inexpensive alloying elements and the use of more efficient heat treatment processes [1-3].

Increasing the efficiency of controlling the processes ensuring the production of high-quality wheel steel requires the development of information and mathematical support based on an adequate connection between the chemical composition of steel and the service properties of metal products.

The effectiveness of solving strategic problems ensuring the competitiveness of metal products in specific industrial conditions is largely determined by the degree of computerization of scientific and technical services and manufacturing areas, the availability of workable information and analytical systems for a comprehensive analysis of current production data.

The methodology of creating and practical use of information-analytical systems [4, 5] being developed in ISI NAS of Ukraine on the basis of databases and models of metal melts is the basis for automating the multidimensional search for optimal solutions.

Modern information technologies allow solving problems with various types of data and obtaining samples for any information that provides the solution of forecasting problems based on complex analysis and interpretation of diverse data.

Taking into account the heat treatment technology, a representative array of experimental data was formed in order to identify the main regularities, the effect of the composition of steel for railroad wheels on the complex of its properties. It includes information on the characteristics of 69 melts of steel of the following grade –T (open-hearth production), ER7 (n=20), ER8 (n=5) and grade –T (n=36), (CCP) under the conditions of PJSC "Interpipe NTRP".

Mechanical properties of steel products and chemical composition of steel for special purposes usually have wide fluctuations, noisiness, and often data incompleteness. In this regard, the concept of assessing the reliability of data was adopted by means of successive elaboration of areas ("microscope" principle) on the basis of a step-by-step analysis of the initial information.

For the purpose of the multidimensional analysis of the data, the mathematical software is generated. Along with the traditional software of the primary data analysis, it includes the original methods of purposeful data projection, searching for hidden regularities on the basis of the methods of physic-chemical modeling of multicomponent metal melts covering a wide range of alloying elements. The use of modern information technologies is an effective tool for solving the problems of optimizing the quality of metal products for a specific purpose.

Presentation of the main materials of the study

To assess the influence of the chemical composition of wheel steel on its mechanical properties and the temperature of phase transformations, the method of physical and chemical modeling developed in ISI NAS of Ukraine has been used. Its principle is to describe the chemical composition of the melt by a complex of integrated model parameters of interatomic interaction characterizing its chemical and structural state.

The implementation of the developed methodology includes [6, 7]:

1. Calculation of the model parameters of the interatomic interaction for a given chemical composition of the charge Z^Y (e) and structural d (10^{-1}nm) states that are defined as the result of a pairwise interaction of all its (m) components by solving a system of nonlinear $m^2 - m + 1$ equations:

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

where $\Delta e'_{ij}$ - the number of electrons that are localized when interacting in the direction of communication $i-j$ at a distance a (along the diagonal of the bcc or fcc lattices), $\Delta e''_{ij}$ - at a distance $d = 0{,}866 \cdot a$ along the face,

$$\Delta e' = (\Delta e'_{12}, \Delta e'_{13}, .\Delta e'_{ij}., \Delta e'_{m-1,m}),$$

$$\Delta e'' = (\Delta e''_{12}, \Delta e''_{13}, .\Delta e''_{ij}., \Delta e''_{m-1,m}) \ .$$

As a result of the solution of the given non-linear system of equations, we determine:

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

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

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

Where n_k - mole fraction, Ru_k^o - the radius of an unpolarized atom, $tg\alpha_k$ - a parameter that characterizes the change in the electron density upon ionization of the atom of the *k-th* component;

2. Construction on the basis of forecast models experimental data for basic mechanical characteristics ($\sigma_в$, δ, HB and etc.) as functions of individual model parameters and their combinations;

3. Determination of the recommended ranges for changing the integral parameters providing the required level of properties.

4. Determination of the chemical composition of steel that meets the required ranges of integral parameters based on optimization methods.

Using integral parameters Z^Y and d as a “convolution” of the chemical composition of a multi-component melt allows increasing the information capacity of models and reducing their parametricity. The regression equations describing their mechanical properties were obtained on the basis of the above experimental data on carbon steels for railway wheels ($r \geq 0.85$):

$$\sigma_в = 2808 + 6685 \cdot Z^Y - 3646 \cdot d$$

$$HB30mm = 2091 + 1502 \cdot Z^Y - 1331 \cdot d$$

$$\delta = 86 \cdot d - 36 \cdot Z^Y - 178$$

The high accuracy of the models allows using the computational experiment methodology to determine the optimal composition of wheel steel. The depen- dence of the strength properties of carbon steels for railroad wheels on the integral charge state parameter Z^Y was used to determine the boundary conditions (Fig.1).

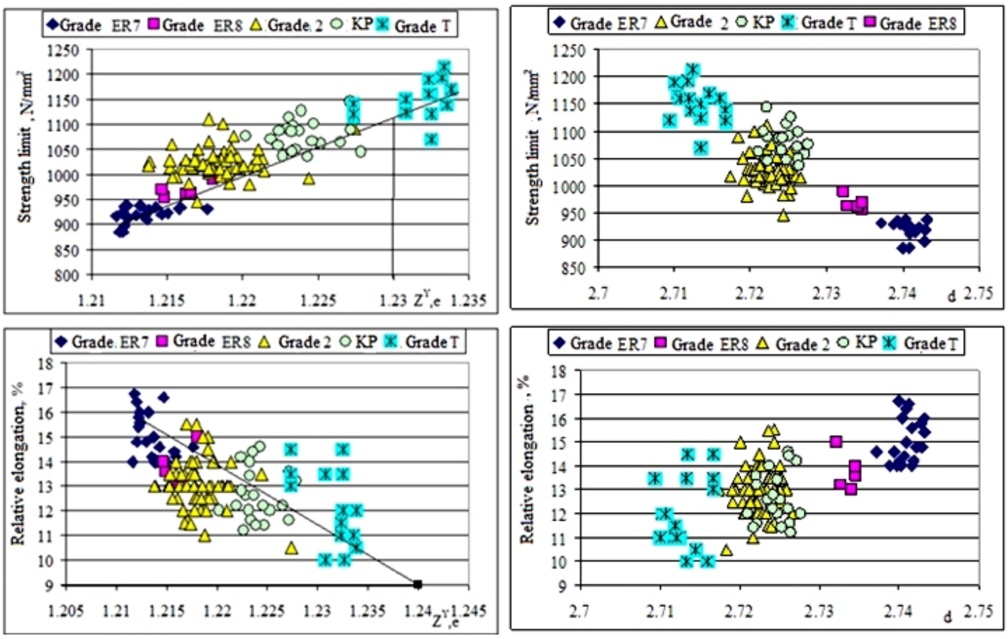

Figure 1. Dependence of mechanical properties of wheel steel grades on model parameters

From Fig. 1 it follows that the change of the parameter $1.235 \leq Z^Y \leq 1.24$ provides the required properties of wheel steel grades. To reveal the influence of elements on the service properties, the steel composition is structured as a chemically unified system that is implemented on the basis of factorial and physico-chemical analyzes dividing them into subsystems - matrix, alloying, micro-alloying and impurity. In case of this approach, the influence of each of the subsystems is considered comprehensively through the physic-chemical parameters of the "convolution" of the chemical composition of each of them, which provides a reduction in the dimension of the forecast models and allows obtaining adequate and stable models in the composition-structure-thermal processing-mechanical properties scheme.

A distinctive feature of the developed model is that not physic-mechanical properties, but a set of corresponding interatomic interaction parameters characterizing the melt and its constituent parts as a chemically unified system are given as optimization criteria. By imposing restrictions on these parameters, it is possible to achieve a certain internal structure of the melt, which, in turn, will provide a given set of mechanical properties.

Fig. 2 shows an example of the results of structuring the chemical composition of steel for railway wheels of the following grades: «2», «T», «ER7», «ER8».

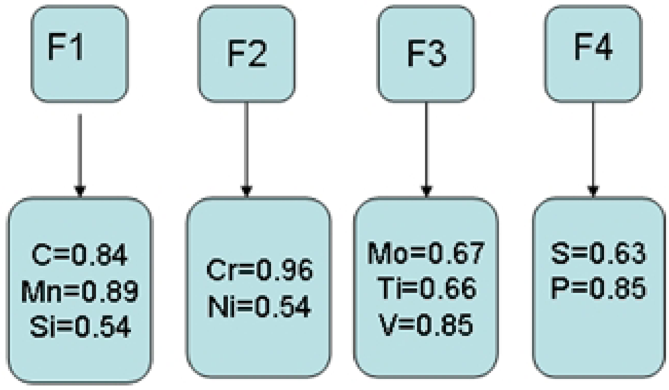

Figure 2. Significant loads of variables on integral factors

On the basis of the identified factors and their corresponding physic-chemical interpretation, the expert makes a decision on the presented options for structuring the choice of model parameters for constructing forecast models and justifying the boundary conditions of optimization parameters. Thus, if the physical meaning of grouping the chemical composition of matrix (factor F1) and impurity (factor F4) subsystems is obvious, then the structure of factors F2 and F3 loaded with impurity micro-alloy elements requires an appropriate interpretation. Significant loads of microalloying elements Cr, Ni and Ti, V, Mo are in accordance with the current data on the physic-chemical properties and reactive ability in solid solutions and melts which are carbon and nitride-forming that explains the logic of their association into one group.

The most characteristic parameters at the heating (cooling) of steel are the critical temperatures of phase transformations (As_1 and As_3). In accordance with the values of the temperature As_1 and As_3, heat treatment modes are also assigned to give the steel the necessary operational properties. To increase the stability of steel to thermal effects, such their alloying is justified, which increases the critical temperature values of austenite transformation and extends the intercritical interval.

On the basis of an analysis of the reference experimental data [8, 9] for predicting the values of critical temperatures and the values of intercritical interval ΔAs using the integral parameters of the interatomic interaction, the following equations were obtained:

$$Ac_3, ^0C = 301480,86 - 96,01Z^Y - 1572,26d - 296435tg\alpha \qquad r = 0.8 \qquad (3)$$

$$\Delta Ac, ^0C = 21255 + 143,55Z^Y - 595,1d - 222770tg\alpha \qquad r = 0.89 \qquad (4)$$

Using the graphical dependencies shown in Fig. 1, as well as the extreme nature of the curves for critical temperatures allows us to determine the boundary conditions for the solution of the problem of selection the optimal composition of the elements of the matrix subsystem from the following ratios :

$$0,8 \le \frac{Si}{Mn} \le 1,0\ , \quad 1,6 \le Si + Mn \le 1,8$$

As it follows from Fig. 3, the required constraint system is corresponded to all the silicon and manganese ratios meeting the boundary conditions determining the widest range of phase transformation temperatures, which ensures the prevention of phase transformations when the rim of the wheel is overheated during braking.

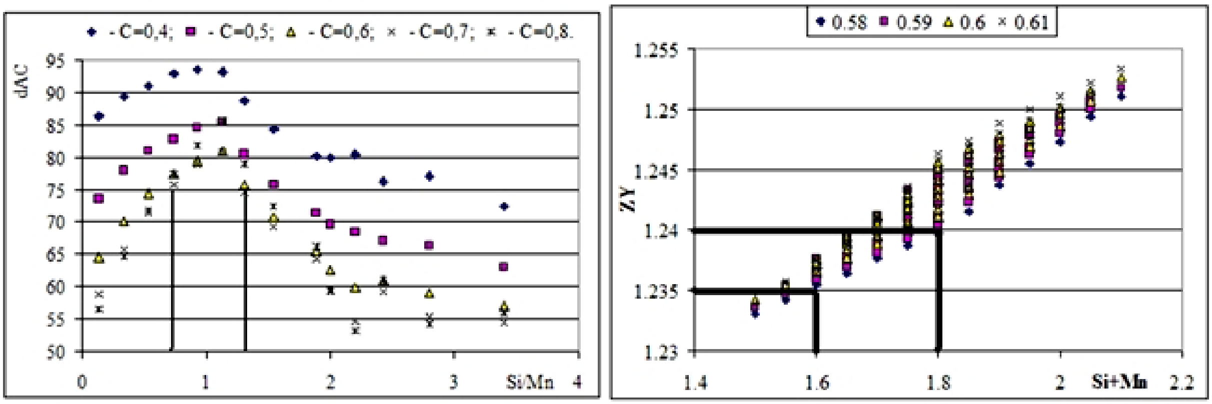

Figure 3. Temperature dependence of phase transformations and the charge state parameter Z^Y of carbon steels for the production of railway wheels on their chemical composition

The solution of the presented inequalities is implemented graphically (Fig. 4). The indicated boundary conditions correspond to values for silicon of 0.7-0.9%; for manganese of 0.8-1.0%.

Limitations on carbon 0.55-0.6 are obtained from a comparative analysis of its effect on the integral parameter Z^Y while ensuring the limitations $1,6 \le Si + Mn \le 1,8$ (Fig.5).

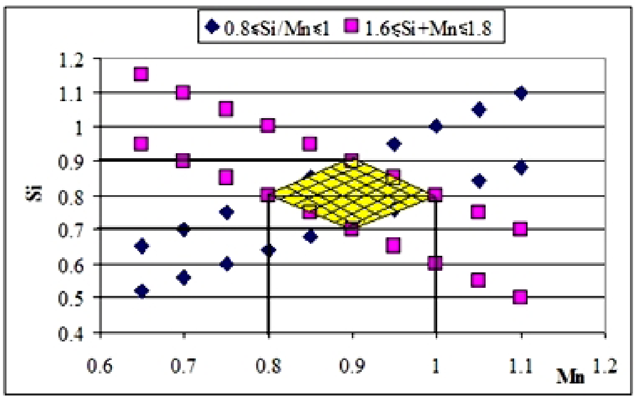

Figure 4. Graphical interpretation of the solution of the ratios $0,8 \le \frac{Si}{Mn} \le 1,0$ and $1,6 \le Si + Mn \le 1,8$

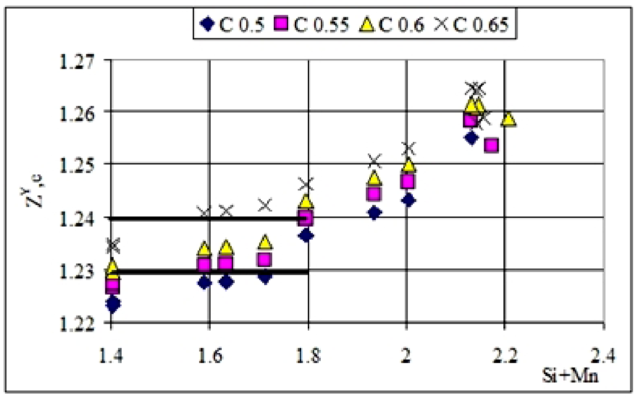

Figure 5. Justification of carbon concentration for specified limits on the indicator Z^Y depending on the content of silicon and manganese

The ranges of the elements of the matrix system obtained during the computational experiment provide the required technological properties: carbon (0.55-0.60%); manganese (0.8-1.0%); silicon (0.7-0.9%).

Fig. 6 shows the relationship between the ultimate strength and the charge state parameter of the subsystem (Mo, Ti, V). As the value of the indicator Z^Y_{MoTiV} increases, the values of the strength limit are reduced.

In the course of the computational experiment (Fig. 7), it has been found that additional vanadium microalloying to 0.08% leads to a decrease in the index Z^Y_{MoTiV} to 1.6e, which, in turn, has a positive effect on the strength properties of steel.

The construction of cartograms of changing the mechanical properties of the steels produced by PJSC "Interpipe NTRP" (Fig. 8) allows us to calculate the prospective area of mechanical properties for steel ER7 additionally alloyed with vanadium.

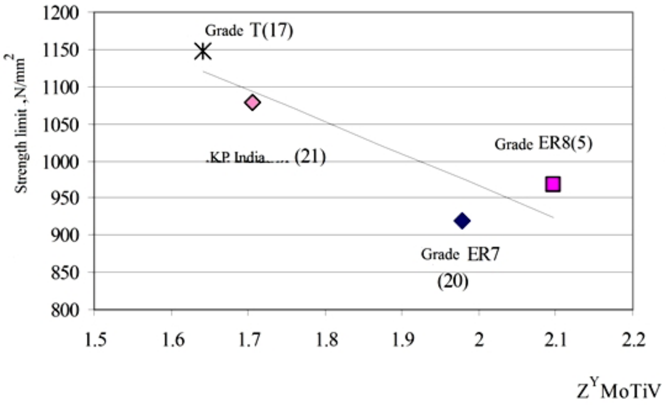

Figure 6. Dependence of the strength limit on the model parameters of the micro-impurity subsystem

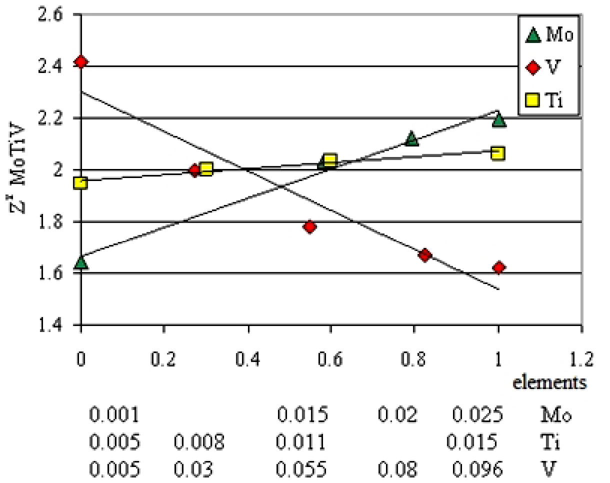

Figure 7. Effect of elements of the impurity-microalloying subsystem Z^Y_{MoTiV} on the change in the parameters of the interatomic interaction

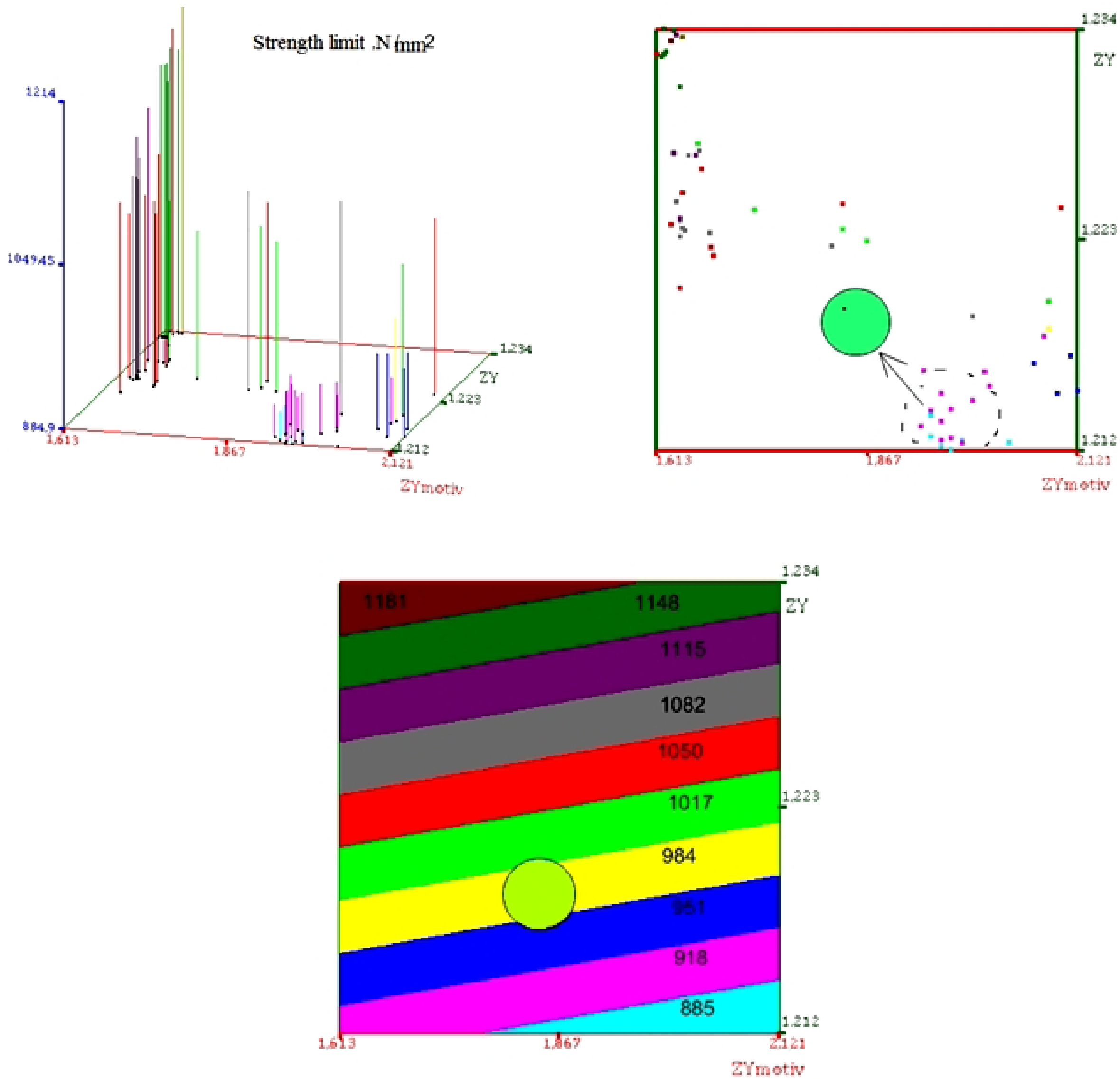

Figure 8. The effect of microalloying of steel ER7 with vanadium

An increase in the thermal stability of steel due to vanadium microalloying forms dispersed carbide or intermetallide phases of high stability, which are not prone to coarsening at elevated temperatures. Vanadium strengthens ferrite more strongly than tungsten and chromium, and approaches the degree of influence on strength to molybdenum. Vanadium makes it difficult to coagulate the carbide phase. The formation of dispersed uniformly distributed carbides containing vanadium and a decrease in the diffusion mobility of carbon atoms due to the presence of vanadium in the solution significantly increase the strength of vanadium steel at elevated temperatures [10]. After the tempering of the steel at temperatures of 400-6600 °C, carbide formation processes develop rather slowly, the carbides VC and Me_7C_3 are present in the form of dispersed precipitates hardening steel. Vanadium is recommended for microalloying as an element that efficiently reduce the grain structure of steel.

Conclusions

1. The method that allows us to reveal hidden patterns of the chemical composition influence on the physic - mechanical properties of the wheel steel at the level of interatomic interaction was proposed.

2. “Narrowed” change ranges of matrix system (C= 0.55-0.60%; Mn= 0.8-1.0%; Si= 0.7-0.9%) providing the required mechanical properties of railway wheels corresponding to GOST 10791-2011 were determined on the basis of laboratory studies, computational experiment and optimization procedures of “Optimization” software complex, as well as graphical interpretation of the obtained dependences on the basis of experimental data on the composition and properties of railway wheels produced in the conditions of PJSC “Interpipe NTRP”.

3. Based on the technique of structuring the total composition of steel (matrix, alloying, microalloying), the influence of elements of the impurity-microalloying subsystem on the formation of strength properties was revealed. The contribution of vanadium, as one of the effective elements of microalloying, in the formation of the strength properties of solid-rolled railway wheels was substantiated.

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