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## QUANTUM MECHANICAL MODEL OF INTERACTION OF CHARGES OF METAL ATOMS DURING CREATION OF CHROME COATINGS

**Purpose.** To determine the dependence of the change in chemical bond energy, using a quantum mechanical model of the interaction of dopant ions with a metal substrate in the form of a chain of N-finite centers located along a straight line.

**Methodology.** Numerical calculation of the analytical expressions of a quantum mechanical system consisting of the interaction between metal ions of doping elements and a chain of N-finite centers.

**Findings.** By solving the Schrödinger equation for a charge moving in the field of a chain with N-finite centers, expressions for calculating the energy of chemical bonding of dopant ions with metal substrates were obtained. The analytical expressions for calculating the energies of chemical bonds are obtained. The most probable types of chemical bonds during the formation of protective coatings under non-stationary temperature conditions were determined.

**Originality.** Schrödinger's equation in ellipsoidal coordinates for the motion of electric charges in a field of N-finite centers located along a straight line was solved and expressions for calculating the energies of chemical bonds were obtained. The solution of the Schrödinger equation is reduced to solving a two-center problem with a perturbation. The model allows us to understand the dynamics of interaction of metal ions with a substrate in the form of chains of atoms. The tendency of change in the energy of chemical bonding of metal ions with substrates depending on the distance between them and the charge value is established.

**Practical value.** The developed method for calculating the energy of chemical bonding between metal ions of alloying elements with a chain of N-finite centers will allow one to qualitatively establish the tendency of formation of certain compounds in the process of obtaining protective coatings under non-stationary temperature conditions. The method can be used to calculate the energies of chemical bonds when selecting alloying elements for other methods of creating protective coatings.

**Keywords:** *carbon steel, chromium plating, alloying, protective coating, modeling, thermodynamics, wear resistance*

**Introduction.** Coatings produced under unsteady temperature conditions (UTC) exhibit distinct and advantageous properties. These coatings are formed through a combination of mechanisms: an applied film similar to gas-phase deposition and an extensive transient diffusion zone akin to diffusion saturation. This hybrid formation process grants UTC coatings superior qualities compared to other coating methods. For example, they can enhance the properties of the applied materials, such as increased wear resistance or improved thermal stability, relative to the substrate. Moreover, UTC coatings demonstrate strong adhesion between powder layers, with particles of one material becoming coated by another. This configuration results in a significantly larger contact surface for chemical reactions, particularly when fine particles are employed. Even micron-sized particles can retain their utility under these conditions. In cases where the particles do not undergo melting, the reactions between the reactants occur through the solid phase via diffusion. Although mass transfer in the solid phase is typically limited, this limitation can be offset by expanding the contact area between reactants. High processing temperatures, which accelerate reaction kinetics, also play a crucial role in this process [1]. Under specific cir-

cumstances, a pure solid flame regime can be achieved, wherein all substances, including intermediate products, remain in a solid state throughout the reaction.

**State of problem.** To enhance the durability and performance of steel, the implementation of hard coatings as protective layers has been employed. These coatings modify the surface properties of the base material, imparting chemical inertness to the surface, which enhances hardness and diminishes wear rates [2, 3]. Among the methods utilized to accomplish this goal, Plasma-Assisted Physical Vapor Deposition (PAPVD) is particularly distinguished. This technique is recognized for the uniform surface it generates and the exceptional mechanical, thermal, and chemical properties it bestows upon the material, acting as an effective shield against corrosion [4].

However, the proposed technology of microwave plasma-enhanced linear antenna CVD is expensive and is not well-suited for protecting the inner surfaces of long piping systems needed for transporting molten materials in nuclear power generation. Additionally, the ultrathin layer (up to 3–5 μm) may not effectively withstand erosive flows in tubulars and other components during material transport. In such conditions, thin coatings may develop micro- and macro-cracks comparable in size to the coating thickness, leading to their degradation and detachment from the metal substrate surfaces

[5]. Moreover, it remains unproven whether these coatings can endure exposure to molten salts. Alternatively, coatings based on metal borides and aluminides, particularly those of iron, chromium, and nickel, can be advantageous when made thicker. These compounds exhibit favorable thermodynamic characteristics and high valence electron densities, forming robust cation-anion bonds in crystalline lattices with a high degree of covalence. According to Zhang, et al. [6], Trolier-McKinstry, et al. [7], and Chen [8], these are the key criteria for creating durable and chemically inert materials.

Over the last two decades, MAX phases have become a promising class of materials attracting researchers. Their properties lie between ceramics and metals: they are less brittle, more heat resistant and have high melting points [9]. Typically, MAX phases present a matrix with carbide inclusions and form a layered hexagonal crystal lattice. Triple and quadruple carbides have an excellent combination of chemical, physical and mechanical properties: high chemical and temperature resistance, low coefficient of thermal expansion, low density, high thermal conductivity and electrical conductivity, low modulus of elasticity, high strength, corrosion resistance in aggressive media and good machinability [10, 11]. Titanium-based MAX phases are of particular interest due to their physical, chemical and mechanical features.

The production of protective coatings through high-temperature synthesis (UTC) involves preparing a powder mixture within an environment conducive to exothermic interactions, which are initiated locally (ignition). This initiation triggers the spontaneous propagation of a reaction front (combustion), followed by the cooling of the resulting synthesized product. Based on the nature of the chemical reactions involved, these processes can be classified into three primary categories: direct synthesis from elemental reactants, direct synthesis from compounds through exchange reactions, and metallothermic processes that incorporate a reduction step. The resulting products encompass a broad spectrum of chemical compounds, including carbides, borides, silicides, nitrides, intermetallics, and chalcogenides.

UTC processes are further categorized based on the physical states of the reactants and products, such as gas-free, low-gas, filtration-based, and metallothermic reactions [12]. The selection of suitable reaction systems follows the principles governing combustion processes. A defining characteristic of these processes is the formation of a target product via an exothermic reaction. In this context, the magnitude of the thermal effect is relevant primarily in ensuring that the combustion can sustain itself, thus enabling efficient synthesis of the desired material. The mechanism of diffusion layer formation is largely influenced by the initial concentration of chromium on the metal surface, which depends on several factors. The diffusion process of chromium across the surface of the material can follow two pathways: either through the formation of stable phases that progressively enrich with chromium or through the creation of higher-order stable phases, followed by the formation of lower- and intermediate-order phases. In the first scenario, the formation of the diffusion layer occurs under equilibrium conditions, while in the second, it follows non-equilibrium conditions. The physico-chemical properties of the diffusion layers formed under these two conditions will differ significantly from one another [13].

Methods for applying protective coatings to metal components vary in terms of coating technology, with the primary objectives being to achieve strong adhesion to the base material and to produce a continuous, non-porous, and environmentally resistant protective layer.

Currently, the main methods for applying protective coatings include electroplating through electrolysis, thermal spraying or metallization, thermal diffusion saturation in powder, immersion in molten metal, and cladding. Depending on the type of bonding between the protective layer and the metal, coatings can be classified into two categories: adhesive coatings and diffusion metallic coatings.

Based on the method used to transfer the diffusing element to the surface being saturated, the primary techniques of diffu-

sion metallization are as follows: immersion in molten metal for elements with a low melting point; saturation from molten salts containing the diffusing element, with or without electrolysis; saturation from the sublimated phase through evaporation of the diffusing element; and saturation from the gas phase (either by contact or non-contact methods) involving halogen compounds of the diffusing element.

**Purpose.** Development and optimization of the technology for obtaining multicomponent chrome coatings designed to improve the performance of press tooling parts at high temperatures

**Methodology.** The process of applying protective coatings under SHS conditions was carried out on a specially designed pilot plant DDTU12. This plant includes not only reaction equipment, but also a system of control and regulation of process parameters, as well as a system of gas utilization, which ensures safe and efficient coating process.

For the application of protective coatings on samples of steel 45, 40X, charge powders were used with different dispersions from 60 to 250 microns. These powders included elements such as chromium, titanium, aluminum oxide, aluminum, ammonium iodide and ammonium chloride. The choice of powder dispersity was guided by studies that showed that the optimum powder fraction to maximize the completeness of the reaction is between 100 and 120  $\mu\text{m}$ .

Compression molding is conducted using a hydraulic vulcanization press, model 100–400 2E, equipped with 400  $\times$  400 mm plates, for processing novel elastomeric materials. These materials are formulated from a copolymer of vinylidene fluoride and hexafluoropropylene, as well as ethylene-propylene rubber. The composites incorporate carbonized polyacrylonitrile (PAN) fibers, granite powder, and aluminosilicate microspheres as reinforcing agents [14, 15]. The press is designed to exert force on the sample while simultaneously applying thermal exposure, facilitating the vulcanization of rubber compounds within molds. With a maximum force capacity of 1,000 kN, this system is crucial for achieving optimal cross-linking in rubber-based composites. These composites have the potential to outperform and eventually supplant conventional materials in various industrial applications, offering several advantages in terms of performance, durability, and material efficiency. For example, rubber-based composites often have a lower density than traditional materials such as metals. This leads to a reduction in the weight of products, which is important in a variety of industries where lightness is a key characteristic. Rubber composites are characterized by shock absorption, flexibility, and elasticity, which makes them capable of handling dynamic loads and adapting to various forms of deformation without losing structural properties. Compared to metals, rubber composites can be less susceptible to corrosion, making them more durable and less costly to maintain in some operating conditions. The ability of rubber to insulate thermally makes them attractive for applications in construction and other industries where thermal insulation is important. The microstructure of structural materials with a protective coating was studied from cross-sections using metallographic microscopes “Neophot-21” and “Neophot-32”. To reveal the microstructure of coatings obtained on steels, a 3% alcohol solution of picric acid in ethyl alcohol was used.

For thermodynamic modeling of chemical reactions in the SHS process, the equilibrium composition of system products was calculated using TERRA. In the development of optimal compositions of powder reaction SHS-charge, providing sufficient coating thickness and high durability, used methods of mathematical planning of the experiment with 3-factor, 3-level composite asymmetric plan of the second order.

**Results.** The mechanism of interaction of charged atomic particles with surface structures can be found by solving quantum-mechanical problems about the influence of external Coulomb potentials on the molecular bonds of the substrate and the motion of electrons in the field of N-Coulomb centers located along a straight line. All these surface structures consist of both separate two-atom bonds and separate linear

atomic chains. The potentials that create charges in these problems will be represented as perturbations to the model Schrödinger equation, and therefore the most accurate solution is possible only in the ellipsoidal coordinate system by solving the Whit-Tecker equation [16, 17].

The use of SHS to create protective coatings requires elucidation of the mechanism of formation of surface layers from the point of view of the interaction of atoms of alloying elements with atoms of the steel substrate, atomic chains and free electrons on its surface. Let us consider the model in which the atoms of the substrate (Fe) are arranged along a straight line and interact with the ions of the basic metals Cr, Ti, Al. Such a model corresponds to a finite linear chain of atoms with distances between atoms  $R$ , and the solution of the multicenter problem is reduced to solving the mathematical model of electron motion in the field of  $N$ -coulomb centers located along a straight line. The Schrödinger equation for a chain of  $N$ -coulomb centers in an ellipsoidal coordinate system is represented as

$$\Delta\Psi + 2[E + U(\lambda, \mu, \varphi)]\Psi = 0, \quad (1)$$

where  $U(\lambda, \mu, \varphi)$  is potential, which we write in the form

$$U(\lambda, \mu, \varphi) = \frac{2}{R} \left[ \frac{Z_1}{\lambda + \mu} + \frac{Z_2}{\lambda - \mu} \right] + \sum \Phi_i(Z_i, \lambda, \mu, \varphi).$$

Considering that  $\Delta$ - Laplace operator in ellipsoidal coordinate systems is expressed by means of the Lamé coefficients

$$\Delta = \left\{ \frac{4}{R^2(\lambda^2 + \mu^2)} \left[ \frac{\partial}{\partial \lambda} (\lambda^2 - 1) \frac{\partial}{\partial \lambda} + \frac{\partial}{\partial \mu} (1 - \mu^2) \frac{\partial}{\partial \mu} \right] + \frac{4}{R^2(\lambda^2 - 1)(1 - \mu^2)} \frac{\partial^2}{\partial \varphi^2} \right\}; \quad (2)$$

$$\Delta = \left\{ \Delta \frac{4}{R^2(\lambda^2 + \mu^2)} \left[ \frac{\partial}{\partial \lambda} (\lambda^2 - 1) \frac{\partial}{\partial \lambda} + \frac{\partial}{\partial \mu} (1 - \mu^2) \frac{\partial}{\partial \mu} \right] + \frac{4}{R^2(\lambda^2 - 1)(1 - \mu^2)} \frac{\partial}{\partial \varphi} \right\};$$

$$\Delta = \frac{4}{R^2(\lambda^2 + \mu^2)} \left[ \frac{\partial}{\partial \lambda} (\lambda^2 - 1) \frac{\partial}{\partial \lambda} + \frac{\partial}{\partial \mu} (1 - \mu^2) \frac{\partial}{\partial \mu} \right] + \frac{4}{R^2(\lambda^2 - 1)(1 - \mu^2)} \frac{\partial}{\partial \varphi}.$$

Then the Schrödinger equation in ellipsoidal co-ordinates will have the form

$$\left\{ \frac{4}{R^2(\lambda^2 + \mu^2)} \left[ \frac{\partial}{\partial \lambda} (\lambda^2 - 1) \frac{\partial}{\partial \lambda} + \frac{\partial}{\partial \mu} (1 - \mu^2) \frac{\partial}{\partial \mu} \right] + \frac{4}{R^2(\lambda^2 - 1)(1 - \mu^2)} \frac{\partial^2}{\partial \varphi^2} \right\} \Psi + 2[E + U(\lambda, \mu)]\Psi = 0; \quad (3)$$

$$\left\{ \frac{4}{R^2(\lambda^2 + \mu^2)} \left[ \frac{\partial}{\partial \lambda} (\lambda^2 - 1) \frac{\partial}{\partial \lambda} + \frac{\partial}{\partial \mu} (1 - \mu^2) \frac{\partial}{\partial \mu} \right] + \frac{4}{R^2(\lambda^2 - 1)(1 - \mu^2)} \frac{\partial}{\partial \varphi} \right\} \Psi + 2[E + U(\lambda, \mu, \varphi)]\Psi = 0;$$

$$\frac{4}{R^2(\lambda^2 + \mu^2)} \left[ \frac{\partial}{\partial \lambda} (\lambda^2 - 1) \frac{\partial}{\partial \lambda} + \frac{\partial}{\partial \mu} (1 - \mu^2) \frac{\partial}{\partial \mu} \right] \Psi + \frac{4}{R^2(\lambda^2 - 1)(1 - \mu^2)} \frac{\partial \Psi}{\partial \varphi} + 2[E + U(\lambda, \mu, \varphi)]\Psi = 0,$$

where  $E$  is electron energy.

For the Coulomb potential we present the solution  $\Psi = X(\lambda)Y(\mu)\Phi(\varphi)$  equation (3), which is divided into three ordinary differential equations of the second order

$$\left[ \frac{\partial^2}{\partial \phi^2} + \Lambda^2 \right] \Phi(\phi) = 0; \quad (4)$$

$$\left[ \frac{\partial}{\partial \mu} (1 - \mu^2) \frac{\partial}{\partial \mu} + \frac{\Lambda^2}{1 - \mu^2} - \mu^2 \varepsilon + \mu Z^+ + A \right] Y(\mu) = 0; \quad (5)$$

$$\left[ \frac{\partial}{\partial \mu} (1 - \mu^2) \frac{\partial}{\partial \mu} + \frac{\Lambda^2}{1 - \mu^2} - \mu^2 \varepsilon + A \right] Y(\mu) = 0;$$

$$\left[ \frac{\partial}{\partial \lambda} (\lambda^2 - 1) \frac{\partial}{\partial \lambda} - \frac{\Lambda^2}{\lambda^2 - 1} + \lambda^2 \varepsilon + \lambda Z^+ - A \right] X(\lambda) = 0; \quad (6)$$

$$\left[ \frac{\partial}{\partial \lambda} (\lambda^2 - 1) \frac{\partial}{\partial \lambda} - \frac{\Lambda^2}{\lambda^2 - 1} - \lambda^2 \varepsilon - A \right] X(\lambda) = 0,$$

where  $F(\varphi) = \exp(i\Lambda\varphi)$ ,  $|\Lambda|$  - integer.

Knowing the basic Schrödinger equations, let us find the potentials created by a linear chain of atoms. Let us imagine that the linear chain of atoms is located along the  $OZ$  axis directed from the charge  $Z_1$  to charge  $Z_i$

$$\Phi_i(Z_i, x, y, z) = \frac{Z_i}{\sqrt{x^2 + y^2 + \left(z - \frac{R_i}{N-1}\right)^2}}, \quad (7)$$

where  $\Phi_i(Z_i, x, y, z)$  is the potential, which is created by the chain of  $N$ -coulomb charges. At transition from Cartesian coordinates to ellipsoidal coordinates  $\Phi_i(Z_i, x, y, z) \rightarrow \Phi_i(Z_i, \lambda, \mu, \varphi)$  we use the relations (1)

$$x^2 = \frac{R^2}{4} (\lambda^2 - 1)(\mu^2 - 1) \cos^2 \varphi; \quad (8)$$

$$y^2 = \frac{R^2}{4} (\lambda^2 - 1)(\mu^2 - 1) \sin^2 \varphi; \quad (9)$$

$$z^2 = \frac{R^2}{4} \left( \lambda^2 + \mu^2 - 1 - \frac{4i}{N-1} \lambda \mu + \frac{4i^2}{(N-1)^2} \right). \quad (10)$$

We substitute (8–10) into (7) and after some simple transformations we obtain

$$\Phi_i(Z_i, \lambda, \mu, \varphi) = \frac{2Z_i}{R(\lambda + \mu)} \left( 1 - \frac{1 + 2\lambda\mu + \frac{4i}{N-1} \lambda\mu + \frac{4i^2}{(N-1)^2}}{\lambda^2 + \mu^2} \right)^{\frac{1}{2}}.$$

Then the potential, which is created by the chain of  $N$ -coulomb charges, has the form

$$\Phi_i(Z_i, \lambda, \mu, \varphi) = \frac{2Z_i}{R(\lambda + \mu)} \left( 1 - \frac{1 + 2\lambda\mu + \frac{4i}{N-1} \lambda\mu + \frac{4i^2}{(N-1)^2}}{\lambda^2 + \mu^2} \right)^{\frac{1}{2}};$$

$$W = \sum_{i=1}^n \frac{2Z_i}{R(\lambda + \mu)} \left( 1 - \frac{1 + 2\lambda\mu + \frac{4i}{N-1} \lambda\mu + \frac{4i^2}{(N-1)^2}}{\lambda^2 + \mu^2} \right)^{\frac{1}{2}}.$$

If we denote

$$\theta^2(\lambda, \mu) = \frac{1 + 2\lambda\mu + \frac{4i}{N-1} \lambda\mu + \frac{4i^2}{(N-1)^2}}{\lambda^2 + \mu^2}, \quad (11)$$

then  $\left[1 - \theta^2(\lambda, \mu)\right]^{\frac{1}{2}} = \Omega(\lambda, \mu)$ , and (11) decompose by Legendre polynomials  $\Omega(\lambda, \mu) = \frac{\pi}{2} \sum_{k=0}^{\infty} (4k+1) \left\{ \frac{(2k-1)!!}{2^k k!} \right\}^2 P_{2k}(\theta(\lambda, \mu))$ ,

then the problem reduces to the solution of the two-center problem with perturbation

$$U(Z_i, \lambda, \mu, \varphi) = \frac{2}{R} \left[ \left( \frac{Z_a}{\lambda + \mu} + \frac{Z_b}{\lambda - \mu} + \sum_{i=2}^{N-1} \frac{Z_j}{\lambda + \mu} \right) + \sum_{i=2}^{N-1} \varphi(\lambda, \mu, \varphi) \right]. \quad (12)$$

From (6) it is well seen that the potential  $U(Z, \lambda, \mu, \varphi)$  is easily reduced to a two-centered potential if we represent  $Z_1 = Z_a$ , a  $Z_2 = \sum_{i=2}^{N-1} Z_i$ , and the perturbation summand that depends on the physical parameters of the circuit [18]

$$\varphi_i(\lambda, \mu, \varphi) = \frac{2Z_i}{R(\lambda + \mu)} g(\lambda, \mu, \varphi, i), \quad (13)$$

where  $g(\lambda, \mu, \varphi, i) = \frac{\pi}{2} \sum_{k=0}^{\infty} (4k+1) \left\{ \frac{(2k-1)!!}{2^k k!} \right\}^2 P_{2k}(\theta(\lambda, \mu))$ .

$$\text{Denote } \chi = -2 - \frac{4i}{N-1} \lambda \mu + \frac{4i^2}{(n-1)^2}.$$

Then we write the perturbation in the form

$$W = \frac{\pi^2}{8R} \sum_{i=2}^{n-1} Z_i \{C_1 I_5 + C_2(\chi) I_3 + C_3(\chi) I_1\}; \quad C_i = f(\chi). \quad (14)$$

Thus, the additive to the total chain energy is a function of charges, the number of atoms, and internuclear distance, and the wave function for the Hamilton equation with potential

$$\begin{aligned} E_{ee} = & \frac{4}{R \left[ \frac{1}{2a} - \frac{4}{3} a \cdot e^{4a} \cdot E_i(-4a) \right]^2} \left[ \left( \frac{3}{40a^2} + \frac{1}{20a^2} \right) \cdot (C + \ln 2a) + e^{8a} E_i^2(-8a) \times \right. \\ & \left. \times \left( \frac{3}{40a^2} + \frac{11}{20a} + \frac{7}{5} + \frac{8a}{15} \right) + e^{4a} E_i^2(-8a) \frac{4a^2}{15} + e^{4a} E_i^2(-4a) \left( -\frac{3}{20a^2} + \frac{1}{2a} - \frac{1}{5} \right) + \frac{1}{8a} - \frac{1}{10} \right]; \\ W_3 = E_0(R_1, R_2, R_3) = & E_0(R_1) + \sum_{i=1}^N \frac{4aZ_3}{R_2 \left[ \frac{1}{2a} - \frac{4}{3} e^{4a} E_i(-4a) \right]} - Q_0^0(\lambda_3) \left[ \frac{2}{3} e^{4a} E_i(-4a) - \frac{1}{4a^2} \right] - \\ & - \frac{1}{8a^2 e^{2a\lambda_3-1}} \left[ P_2(\lambda_3) P_2(\mu_3) - 1 \right] e^{2a(\lambda_3+1)} E(-2a(\lambda_3+1)) - \\ & - e^{2a(\lambda_3-1)} E_i(-2a(\lambda_3-1)) - Q_2(\lambda_3) P(\mu_3) \left[ \frac{2}{3} e^{4a} E_i(-4a) + (\lambda_3^2-1) e^{2a(\lambda_3-1)} E_i(-2a(\lambda_3-1)) \right] + \\ & + Q_0(\lambda_3) P_2(\lambda_3) P_2(\mu_3) e^{-2a(\lambda_3-1)} \left[ (\lambda_3^2-1) e^{2a(\lambda_3+1)} E_i(-2a(\lambda_3+1)) - \left( \frac{1}{2a} - \frac{1}{4a^2} - \frac{\lambda_3}{2a} \right) \right] \times \\ & \left. \times P_2(\lambda_3) P_2(\mu_3) \left[ e^{4a} E_i(\lambda_3+1) E_i(-2a(\lambda_3+1)) + \frac{1}{2a} e^{-2a(\lambda_3-1)} \right] \right\}. \end{aligned} \quad (16)$$

Theoretical calculations showed good agreement with experimental values. It is shown that mainly Fe-Cr, Fe-Al, Cr-Ti and Al-Ti compounds are formed on the surface of the iron matrix, since they have lower bonding energy.

If Al leaves as oxides, only Fe-Cr and Cr-Ti remain. The amount of alloying compounds also depends on the initial composition. The probability of formation of other phases is much lower because their chemical bonding energy is higher (Table 1).

Thermodynamic process modeling involves a comprehensive thermodynamic analysis of the equilibrium states within a system. These systems are defined as isolated material regions whose interactions with their surroundings are limited to the transfer of heat and mechanical work. The evaluation of thermodynamic equilibrium in complex systems – entailing the determination of equilibrium parameters, thermodynamic characteristics, and both chemical and phase compositions – is conducted by minimizing the isobaric-isothermal potential or maximizing the system's entropy. This process considers all individual substances that could potentially coexist in equilibrium, ensuring an accurate representation of the system's behavior under specified conditions.

The kinetic regularities of the chemical processes in the SHS depend on both the temperature and the diffusion factors. Assuming that at the stage of heating the inhibition of the diffusion processes in the gas phase is small, and the rate of change

$U(Z, \lambda, \mu, \varphi)$  without  $\varphi_i(Z_i, \lambda, \mu, \varphi)$ , is a function of the physical parameters of the system.

Now we will calculate the potential curves using the formalism of the two-center problem

$$E = E_{k,\varepsilon,n} + E_{ee} + W_3 + W + \sum_{i=1}^N \sum_{j=1}^N \frac{Z_i Z_j}{R_{ij}}, \quad (15)$$

where  $W_3$  – perturbation created by metal ions,  $E_{8e}$  – magnitude of electron-electron interactions, a  $\sum_{j=1}^N \sum_{i=1}^N \frac{Z_i Z_j}{R_{ij}}$  – coulomb interactions. Then we will use the following equations

$$E_{\frac{1}{2},0,0} = \frac{4 \left[ \frac{1}{2} (a - Z^+) + e^{4a} E_i(-4a) \left( a^2 - aZ^+ - \frac{1}{4} a \right) \right]}{R^2 \left[ \frac{1}{2a} - \frac{4}{3} a e^{4a} E_i(-4a) \right]},$$

where  $a = -1 + \sqrt{0.5 + (Z_1 + Z_2)R}$ , but  $E(-4a)$  – integral exponential.

in temperature in comparison with the rate of flow of gas-phase chemical reactions is small, it can be assumed that at each temperature the equilibrium composition of the reaction products is determined. In this case, by calculating the equilibrium composition of the reaction products for a number of temperatures, we can trace the chemical picture of the process.

Table 1

Calculation of chemical bonding parameters of interacting metals

No.	Chemical bonding	Length of the chemical bond, Å	Chemical bonding energy, a.e.
1	Fe-Fe	2.268	-0.154
2	Fe-Cr	2.277	-0.138
3	Fe-Ti	2.448	-0,166
4	Fe-Al	2.421	-0.136
5	Cr-Cr	2.286	-0.128
6	Cr-Ti	2.459	-0.139
7	Cr-Al	2.431	-0.121
8	Al-Ti	2.601	-0.148
9	Ti-Ti	3.244	-0.178

Factors for the Ti-Cr system

Characteristic	Factors		
	CrC %, wt.	Ti %, wt.	Cr %, wt.
Code	$X_3$	$X_2$	$X_1$
Basic level	20	20	5
Variation interval	5	5	2
The lower level	15	15	7
The upper level	25	25	3

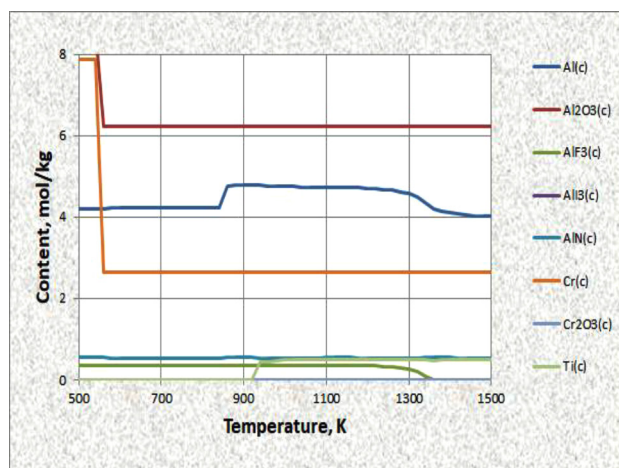


Fig. 2. Distribution of condensed products in the reactor for the Cr-Ti system

The existence of limiting temperatures at which the combustion front can propagate imposes certain constraints on the utilization of the combustion mode in technological processes. In contrast, the thermal autoignition mode does not suffer from these restrictions, allowing for greater flexibility. By diluting the initial powder mixture with an inert substance to approximately 85–90 % of the mass, it becomes feasible to lower the peak process temperature to a level suitable for specific technological requirements.

As the temperature increases, the proportion of products in the gaseous phase rises, accompanied by the release of condensed products. In the temperature range of 400–1,600 K, the share of the condensed phase diminishes due to the vaporization of carriers used in the system. Notably, at temperatures starting from 800 K, decomposition reactions begin, leading to the generation of decomposition products and a sharp escalation in the number of gas molecules.

The gaseous reaction products interact with the powder system elements such as aluminum (Al), titanium (Ti), and chromium (Cr), chromium component (CrC), causing them to transition into the gas phase in forms such as AlJ, AlJ<sub>2</sub>, AlCl, AlCl<sub>2</sub>, CrCl<sub>2</sub>, CrF, CrF<sub>2</sub>, CrF<sub>4</sub>, TiCl<sub>2</sub>, TiCl<sub>3</sub>, TiCl<sub>4</sub>, and others. At temperatures above 800 K, the fraction of the condensed phase stabilizes, indicating that reactions in the range of 800–1,600 K proceed with the release of condensed products without altering the overall number of molecules. This is characteristic of decomposition, disproportionation, or exchange reactions occurring with the substrate, which form the basis of chemical transport processes of elements within the system.

To optimize the composition of the powder charges, a mathematical design of experiments was conducted. The experimental factors included ( $X_1$ ) the content of alloying elements (chromium compounds), ( $X_2$ ) the content of titanium, and ( $X_3$ ) the chromium component content. The selected optimization parameter was  $Y_1$ , which represented the wear resistance indicator of the Cr-Ti system (as presented in Table 2).

When obtaining multi-component chromium coatings alloyed with titanium, the coating consists of several distinct phases, including  $(\text{FeCr})_{23}\text{C}_6$  and the  $\text{Fe}_2\text{Al}_5$  aluminide alloyed with chromium and titanium, along with  $\text{Cr}_2\text{Ti}$  inclusions. Additionally, an ordered solid solution of  $\text{Fe}_3\text{Al}$ , alloyed with Cr and Ti, is present, as well as an  $\alpha$ -solid solution containing Al, Cr, and Ti in the Fe matrix. These phase compositions contribute to the overall performance and wear resistance of the coating system.

A thermodynamic system is defined as a conceptual region of matter where interactions with the external environment are confined to the transfer of heat and mechanical work. Advanced thermodynamic modeling techniques enable the quantitative analysis and prediction of the behavior, composi-

tion, and properties of intricate, heterogeneous, multicomponent, and multiphase systems over extensive temperature and pressure ranges, while considering both chemical reactions and phase transitions. This methodology allows for a thorough investigation of thermochemical processes in high-temperature installations, enhancing operational efficiency, predicting the outcomes of high-temperature interactions, and significantly reducing the time and costs associated with experimental research. Additionally, it facilitates the structured integration of theoretical insights and experimental findings.

The computation of thermodynamic equilibrium within any given system entails determining all equilibrium parameters, thermodynamic variables, and phase compositions by minimizing the isobaric-isothermal potential or maximizing entropy. These calculations incorporate all potential substances that could be present in equilibrium, ensuring a comprehensive analysis of the system's behavior under defined conditions.

The choice of the basic level and the intervals of variation is made on the basis that the introduction of ChC less than 10 wt. Based on the study of the change in the characteristic temperatures of the SHS process, the number of ChC is selected.  $\text{Al}_2\text{O}_3$  is used as a ballast impurity to produce a one hundred percent composition of the powder SHS charges.

The obtained equation characterizing the influence of the technological regime and the composition of the charge on the parameters of optimization of physical, mechanical and operational properties, have the following form  $Y_1 = 86 - 2.2X_1 - 3.3X_2 + 0.4X_3 - 4X_1^2 + 0.5X_2^2 + 5X_3^2 - 0.875X_1X_2 - 2.125X_1X_3 - 0.125X_2X_3$ .

The response surface of the obtained mathematical models is represented by three-dimensional graphical dependencies (Fig. 4).

Coatings do not contain the brittle FeAl phase, which is present in all coatings obtained under isothermal conditions, which can be explained by the high rate of temperature rise at the stage of thermal spontaneous combustion. This is typical for the processes of electric heating and high-frequency current processing.

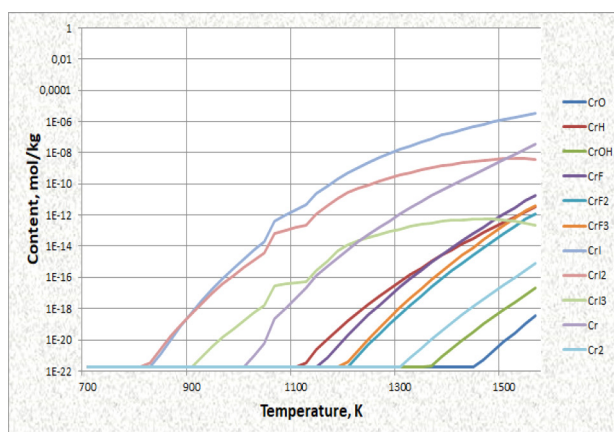


Fig. 3. Distribution of gaseous chromium compounds in the reactor for the Cr-Ti system

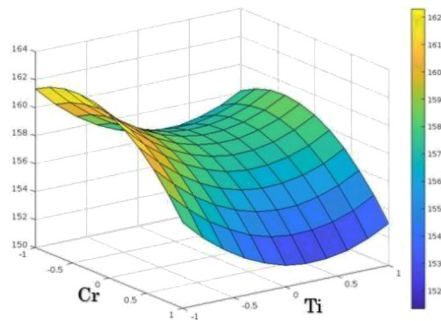


Fig. 4. Influence of Ti and Cr on the wear resistance of coatings in the Cr-Ti system

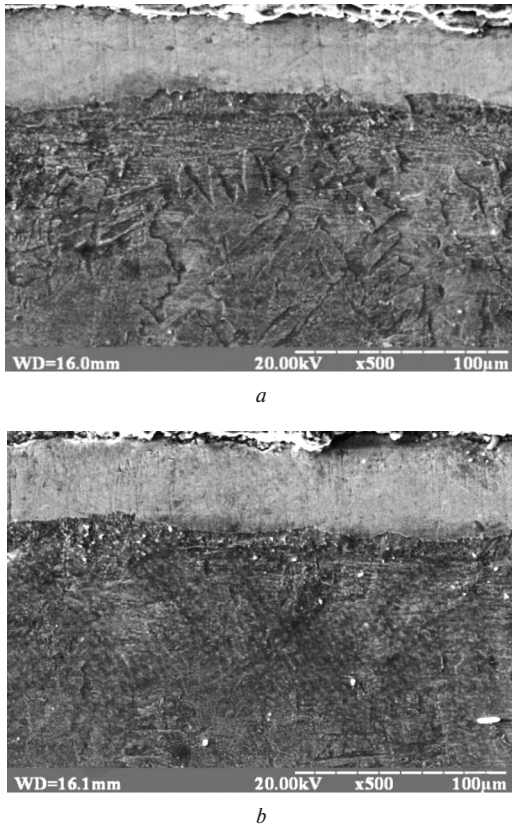


Fig. 5. Protective chrome coatings alloyed with titanium ( $t_p = 1,000^\circ\text{C}$ ,  $\tau_p = 30$  min): a – steel 45; b – steel 40X. (Magnification: 500)

**Conclusions.** The high efficiency of the developed technology of multi-component chromium plated coatings, confirmed both experimentally and theoretically, was achieved during the research. The coatings obtained by this technology demonstrated excellent characteristics in terms of wear resistance and thermal stability. On the samples of steel 45 and 40X improved performance properties were achieved compared to traditional coatings, which manifested itself in a significant reduction of wear at high temperatures and aggressive environments.

The multi-component chrome coatings demonstrated high mechanical properties such as hardness and shear strength due to the optimized composition and application technology. The theoretical calculations carried out showed good agreement with the experimental values. It is shown that mainly Fe-Cr, Fe-Al, Cr-Ti and Al-Ti compounds are formed on the surface of iron matrix because they have lower bonding energy. If Al leaves as oxides, only Fe-Cr and Cr-Ti remain. The amount of alloying compounds also depends on the initial composition. Calculations of thermodynamic equilibrium of reaction products and kinetic regularities confirmed the possibility of

obtaining coatings with specified properties at different temperature regimes. Modeling showed that the selected powder mixtures and technological parameters provide effective formation of protective layers.

Metallographic analysis showed high quality and homogeneity of the coatings, their good adhesion to the steel substrate and resistance to cracks and defects. The technology was successfully applied for protection of press tooling parts operating under conditions of extreme temperatures and aggressive environments of rubber production.

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## Квантово-механічна модель взаємодії зарядів металічних атомів при створенні хромованих покриттів

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**Мета.** Встановити за допомогою квантово-механічної моделі взаємодії іонів легуючих атомів із металевою підкладкою у вигляді ланцюга N-фінітних центрів, що розміщені вздовж прямої, залежність зміни енергії хімічного зв'язку.

**Методика.** Чисельний розрахунок аналітичних виразів квантово-механічної системи, що складається зі взаємодії між металевими іонами легуючих елементів з ланцюгом N-фінітних центрів.

**Результати.** Шляхом розв'язання рівняння Шредінгера для заряду, що рухається в полі ланцюгу з N-фініт-

ними центрами, отримані вирази для розрахунку енергії хімічного зв'язку іонів легуючих атомів з металевими підкладками. Отримані аналітичні вирази для розрахунку енергії хімічних зв'язків. Встановлені найбільш імовірні типи хімічних зв'язків під час отримання захисних покриттів при нестационарних температурних умовах.

**Наукова новизна.** Розв'язане рівняння Шредінгера в еліпсоїдальних координатах для руху електричних зарядів у полі N-фінітних центрів, що розміщені вздовж прямої, та отримані вирази для розрахунку енергії хімічних зв'язків. Розв'язок рівняння Шредінгера звівся до розв'язку двоцентрової задачі зі збуренням. Модель дозволяє зрозуміти динаміку взаємодії металевих іонів із підкладкою у вигляді ланцюгів атомів. Встановлена тенденція зміни енергії хімічного зв'язку металевих іонів з підкладками в залежності від відстані між ними й величини заряду.

**Практична значимість.** Розроблена методика розрахунку енергії хімічного зв'язку між металевими іонами легуючих елементів з ланцюгом N-фінітних центрів дозволить якісно встановлювати тенденцію утворення тих чи інших сполук при отриманні захисних покриттів при нестационарних температурних умовах. Метод може бути використаний для розрахунку енергії хімічних зв'язків під час вибору легуючих елементів за інших методів створення захисних покриттів.

**Ключові слова:** вуглецева сталь, хромовання, легування, захисне покриття, моделювання, термодинаміка, зносостійкість

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