SECTION 3
FILM MATERIALS AND COATINGS

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QUANTUM MECHANICAL MODEL OF INTERACTION BETWEEN IONS OF DOPING ATOMS OF HIGH-PURE METALS

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Using a quantum mechanical model of the interaction of ions of dopant atoms of pure metals with a metal substrate in the form of a chain of N-finite centers, it has been established that they are located along a straight line. This allows us to establish a tendency for the formation of certain high-purity compounds when obtaining protective chrome coatings formed under non-stationary temperature conditions. The non-equilibrium processes characteristic of such coating formation modes cause the intensive emergence of a wide range of phases and compounds that enrich functionally active systems and give them increased structural complexity. By solving the Schrödinger equation for a charge moving in a field of a chain with N-finite centers, expressions were obtained for calculating the chemical bond energy of dopant ions. It has been established that the energy of chemical interactions directly depends on the individual characteristics of high-purity elements, which contribute significantly to the formation of the final properties of materials.

INTRODUCTION

High-purity metals are widely used in modern technology and the national economy: nuclear power, electronic, aerospace, medicine, defence, and military industries, as well as in fundamental scientific research. The fields of application of high-purity rare metals are constantly expanding. The development trend of modern science and technology requires high-purity or ultra-high-purity of metals, because some important characteristics of metals are affected by the type and amount of impurities in the matrix, and some characteristics are even masked by trace elements [1, 2].

Coatings synthesized under unsteady temperature conditions (UTC) demonstrate a complex set of unique and technologically valuable properties. Their formation mechanism can be considered hybrid in nature, as it integrates features of two classical approaches: on the one hand, the process resembles gas-phase deposition, where a thin external film is applied, and on the other hand, it incorporates a pronounced transient diffusion zone characteristic of diffusion-based saturation techniques. Such a dual mechanism leads to the generation of multilayered and structurally heterogeneous coatings, endowing them with performance characteristics that surpass those achieved by conventional coating technologies [3, 4].

A particularly important advantage of UTC coatings is their capacity to significantly enhance the operational properties of the substrate material. Depending on the system employed, these coatings provide increased resistance to wear, improved thermal and chemical stability, as well as prolonged service life of the treated component. At the microstructural level, the coatings exhibit excellent adhesion between adjacent powder layers, which is facilitated by the phenomenon wherein particles of one constituent material are effectively enveloped by another [5, 6]. As a result, the effective surface area available for interfacial chemical interaction increases substantially. This effect is especially pronounced when fine powders are used, since even micron-sized particles remain reactive under UTC processing conditions.

When particle melting does not occur, chemical transformations proceed predominantly through solid-state diffusion mechanisms. Although diffusion in the solid phase is inherently limited in rate, this drawback is mitigated by the dramatic increase in the contact surface between reactants within the composite medium. Elevated processing temperatures, which accelerate diffusion and reaction kinetics, serve as an additional factor promoting the formation of continuous and thermodynamically stable coatings. Under certain regimes, the system may enter a “solid flame” mode, in which all reactants and intermediate products remain in the condensed phase throughout the reaction, thereby ensuring the stability and homogeneity of the coating structure [7, 8].

Synthesis of protective coatings based on chromium with light elements (Al, B, C, Si) is associated with significant obstacles in the formation of specified structures. This raises the problem of improving experimental methods for obtaining coatings under non-stationary temperature conditions with the necessary set of physicochemical properties [9–11].

Currently, the prediction of coating properties is done rather intuitively based on a large number of studies. However, this mechanism does not always give the desired results, and in some cases, it gives negative results. Therefore, there is a problem of developing a theory of the formation of coatings based on chromium with light elements using microscopic theories of substance formation. Such theories include quantum mechanics, which allows calculating energies, lengths of chemical bonds, and the influence of ions of other elements on them. When synthesizing coatings under

non-stationary temperature conditions, problems arise due to the dependence of the process and its duration on a number of parameters, such as the heterogeneity of the particle size distribution of the powder working mixture, the uneven distribution of particles by size, the heterogeneity of the distribution of voids in the reaction zone volume, and spatial fluctuations in the combustion temperature, which leads to the formation of chemical compounds with significant variations in composition. Therefore, further analysis will focus on the simplest chemical compounds with the calculation of the lengths and energies of chemical bonds in selected systems [12].

EXPERIMENTAL RESULTS AND DISCUSSION

Thermodynamic modeling of processes is based on a comprehensive analysis of the equilibrium states of multicomponent systems, which are considered as conditionally isolated material regions whose interaction with the external environment is limited only to the exchange of heat and mechanical work. The determination of the conditions of thermodynamic equilibrium of arbitrary systems, as well as the calculation of their phase and chemical composition, is carried out by minimizing the isobaric-isothermal potential or, in an equivalent formulation, by maximizing entropy, taking into account the possible existence of all potentially stable phases and chemical compounds. This approach allows not only to evaluate the parameters of the equilibrium state, but also to establish a set of thermodynamic characteristics necessary for predicting the direction and possibility of the course of processes.

At the same time, the kinetic patterns of chemical reactions are determined not only by the temperature factor, but also by the conditions of diffusion interaction between the reacting components. Assuming that during the heating stage, diffusion inhibition in the gas phase is insignificant, and the rate of temperature change is significantly lower than the rate of gas-phase chemical reactions, it can be assumed that for each fixed temperature value, a corresponding equilibrium composition of products is formed. Thus, a sequential calculation of the equilibrium composition for a range of temperatures makes it possible to reconstruct the overall picture of chemical transformations and evaluate their dynamics during the heating process.

The existence of critical temperature limits at which the combustion front can spread plays a special role in the practical application of thermodynamic modeling. This feature imposes significant restrictions on the use of the combustion mode in technological schemes. In contrast, the thermal self-ignition mode is not characterized by such limitations, which makes it more flexible in terms of technological implementation. In particular, the introduction of an inert additive in the amount of about 45…50% of the mass into the initial powder mixture allows to significantly reduce the peak values of the process temperature, adjusting them to the level optimal for specific technological conditions and requirements.

For the purposes of this research, Cr compounds with light elements B, C, Al, and Si. Numerous researches have shown that during the process of applying coatings to the surface of iron, a number of chemical compounds are formed: Cr, CrB, Cr_3B_4, CrB_2, Cr_5B_3, $AlCr_2$, $Cr5Al_8$, Al_9Cr_4, Cr_3C_2, Cr_7C_3, $Cr_{23}C_6$, CrSi, $CrSi_2$, Cr_3Si, Cr_5Si_3, and other compounds [13]. In addition to two-component compounds, there may also be other multicomponent compounds. The X-ray diffractogram shows compounds whose content exceeds 1% (Fig. 1).

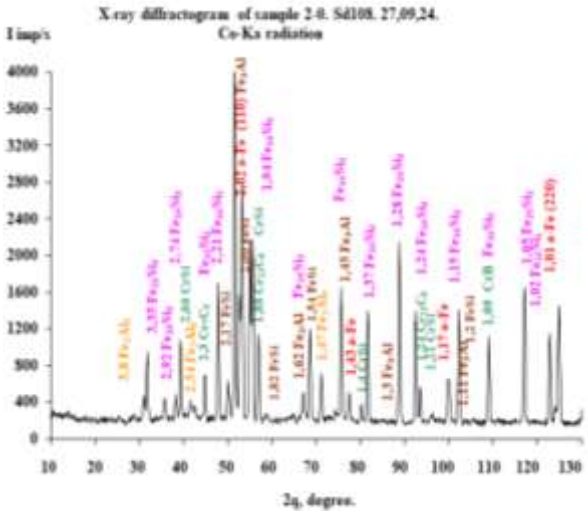

Fig. 1. Diffraction pattern of an iron sample with Cr, B, C, Al, and Si coating

However, to determine the trends in the formation of certain compounds, we will calculate the interatomic distances between simple atoms and their binding energies. The interaction between particles under non-stationary temperature conditions is determined by significant short-range forces that manifest themselves during collisions and significant temperature differences. We will assume that previous collisions and interactions do not affect subsequent ones. For this type of interaction, the most likely are the Coulomb potential and the potential of the oscillatory motion of atoms a and b. At low temperatures, the electrostatic Coulomb interaction has a significant interaction radius.

To construct a physical model of a chemical bond, we will define the potential energy of the interaction of atoms as a function of the charges of the atomic nuclei Z_a and Z_b, the distances between them – r, and the frequencies of the main oscillations of the atoms – γ, which are responsible for the temperature. Using this methodology, it is necessary to solve the problem of electron motion in the field of two oscillating Coulomb centers. If, in an ideal state, the nuclear charges are integer, then due to the fact that these charges surround electrons, which screen the charges and make them effective, i.e., small. The process of obtaining coatings under non-stationary temperature conditions involves charged atoms in neutral, charged, and ionized states, which are in different quantum states characterized by spins s ($s = \frac{1}{2}$, $s = \frac{3}{2}$, $s = \frac{5}{2}\cdots$). When solving the Schrödinger equation, we will assume that the potential energies of the Coulomb potential and the oscillatory

motion potential are added according to the principle of field superposition and do not depend on each other. In this case, the formation of the ferrite structure begins at a plasma temperature of about 3000…5000 K. At this temperature, all atoms are in complete or partial ionization. As the plasma cools, chemical bonds are formed, followed by structures with minimal interaction energy. We will consider the further completion of the structures as the addition of other atoms to the chemical bonds, which affect the chemical bonds in the form of the influence of third charged centers.

To explain the mechanism of formation To explain the mechanism of formation of chemical bonds, it is necessary to solve a number of quantum mechanical problems, in particular to study the motion of an electron in the field of two Coulomb centers, analyze the electron-electron interactions of electrons that form chemical bonds, and evaluate the influence of Coulomb charges of foreign centers on the stability of these bonds.

The total energy of a single chemical bond can be calculated using the formula:

$$E = E_{\frac{1}{2},0,0} + E_{e-e} + W_3 + E_{coul}\,, \qquad (1)$$

where $E_{\frac{1}{2},0,0}$ – energy of the chemical bond in the ground state; E_{e-e} – energy of electron-electron interactions; W_3 – perturbation affecting chemical bonds, and E_{coul} – energy of Coulomb interaction.

To solve these problems, we will use the Schrödinger equation for an electron located in a field of two oscillating Coulomb centers, which has the following form [9–11]:

$$\Delta\Psi + 2[E + U(r_1, r_2) + V_A]\Psi = 0, \qquad (2)$$

where $U(r_1, r_2)$ – potential energy operator of Coulomb centers 1 and 2; V_A – potential that creates the oscillatory motion of nuclei *a* and *b*; Ψ – wave function; Δ – Laplace operator in ellipsoidal coordinate systems, which is expressed using Lamé coefficients [9–11]:

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

where r_a and r_b distances from the electron to centers *a* and *b*. Let us denote the distance between the potential centers by R, then equation (2) in ellipsoidal coordinates will have the form:

$$\left\{\frac{4}{R^2(\lambda^2-\mu^2)}\left[\frac{\partial}{\partial\lambda}(\lambda^2-1)\frac{\partial}{\partial\lambda} + \frac{\partial}{\partial\mu}(1-\mu^2)\frac{\partial}{\partial\mu} + \frac{4}{R^2(\lambda^2-1)(1-\mu^2)}\frac{\partial^2}{\partial\phi^2}\right]\right\}\Psi + 2\left[E - V_{кул} + V_A\right]\Psi = 0, \qquad (3)$$

where $V_{coul} = \frac{2Z_1}{R(\lambda-\mu)} + \frac{2Z_2}{R(\lambda+\mu)}$; $V_A = \gamma((\lambda^2+\mu^2)(R_1^2+R_2^2) + 2\lambda(R_1R_2^2 + R_1^2R_2) + 2R_1R_2)$; E – electron energy; R_1 and R_2 amplitudes of displacement of atoms *a* and *b* from their equilibrium positions.

Choice of an ellipsoidal coordinate system is related to the fact that the Coulomb and oscillatory potentials are separated in it. To solve equation (3), it is necessary that the variables λ and μ in the potential functions are separated and the following condition is satisfied:

$$U(\lambda,\mu)(\lambda^2-\mu^2) = \phi_1(\lambda) - \phi_2(\mu).$$

For Coulomb and oscillatory potentials, we present the solution to equation (3) as $\Psi = X(\lambda)Y(\mu)\cdot\Phi(\phi)$, which is divided into three ordinary second-order differential equations [11, 12]:

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

$$\left[\frac{\partial}{\partial\mu}(1-\mu^2)\frac{\partial}{\partial\mu} + \frac{\Lambda^2}{1-\mu^2} - \mu^2\varepsilon + \mu Z^+ - \left(\frac{R^2E}{2} + \frac{R^2R_1^3}{\gamma}\right)\mu^2 + \frac{R^2\gamma}{2}\mu^4 - A\right]Y(\mu) = 0, \qquad (5)$$

$$\left[\frac{\partial}{\partial\lambda}(\lambda^2-1)\frac{\partial}{\partial\lambda} - \frac{\Lambda^2}{\lambda 2\ -1} + \lambda^2\varepsilon + \lambda Z^+ - \left(\frac{R^2E}{2} + \frac{R^2R_1^3}{\gamma}\right)\mu^2 + \frac{R^2\gamma}{2}\mu^4 - A\right]X(\lambda) = 0, \qquad (6)$$

where $\Phi(\phi) = exp(i\Lambda\phi)$, $|\Lambda|$ – integer; $\varepsilon = \frac{ER^2}{2}$; $Z^{(\pm)} = (Z_a \pm Z_b)R$; *A(R)* – separation constant.

Let us calculate some states using the formula:

$$E_{k,\Lambda,n} = \frac{\langle\Psi_{k,\Lambda,n}|H_0|\Psi^*_{k,\Lambda,n}\rangle}{\langle\Psi_{k,\Lambda,n}|\Psi^*_{k,\Lambda,n}\rangle},$$

where H_0 – Hamiltonian of a two-center problem, and k, Λ, n – are quantum numbers:

$$\hat{H} = \sum_{i=1}^{\infty}\left(-\frac{1}{2}\Delta_i - \frac{Z}{r_i}\right) + \frac{1}{r_{12}},$$

and $\Psi_{k,\Lambda,n}$, $\Psi^*_{k,\Lambda,n}$ – wave functions that are solutions to the Whittaker equation [14]:

$$E_{\frac{1}{2},0,0} = \frac{4\left[\frac{1}{2}(a-Z^+)+e^{4a}E_i(-4a)(a^2-aZ^+-\frac{1}{4}a\right]}{R^2\left[\frac{1}{2a}-\frac{4}{3}ae^{4a}E_i(-4a)\right]}. \qquad (7)$$

To determine trends in the calculation of chemical bonds, we will limit ourselves to spin s=1/2. If chemical bonds have more than one electron, electron-electron interactions must be taken into account. We will calculate electron-electron interactions using the Slater determinant [15]:

$$\Psi\begin{vmatrix} u_1(1) & u_2(1) \\ u_2(2) & u_2(2) \end{vmatrix}_{det}, \qquad (8)$$

where $u_1 = \alpha_0\phi^{(mod)}$; $u_2 = \beta_0\phi^{(mod)}$, i.e., we used the model two-center function of the H_2^+, a $\frac{1}{r_{1,2}}$ as the basis, which can be represented in the form of a Neumann expansion [9–11]:

$$W_1(\lambda,\mu,\phi,\bar{e}) = \frac{2}{R}\sum_{p=0}^{\infty}\sum_{m=-p}^{p}(-1)^m(2p+1)\left[\frac{(p-|m|)!}{(p+|m|)!}\right]\times \times P_p^{|m|}(\lambda_<)Q_p^{|m|}(\lambda_>)P_p^{|m|}(\mu_3)Q_p^{|m|}(\mu_3)e^{im(\phi-\phi_3)}, \qquad (9)$$

where $\lambda_3 = \frac{R_2+R_3}{R_1}$; $\mu_3 = \frac{R_2-R_3}{R_1}$; $R_1 = R$; $R_2 -$ distance from atom 1 to the electron in the bond; $R_3 -$ distance from atom 2 to the electron in the bond; $\lambda_{\lessgtr}$ – greater or lesser of the values; $P_p^{|m|}(\lambda_<)$ and $Q_p^{|m|}(\lambda_>)$ of the attached Legendre functions of the first and second kind [9–11]:

$$E_{e-e} = \left\langle \psi \left| \frac{1}{r_{1,2}} \right|^{*}_{det\,det} = \frac{4}{R\left[\frac{1}{2a} - \frac{4}{3}a \cdot e^{4a} \cdot E_i(-4a)\right]^2} \right\rangle \text{x}$$
$$\left[\left(\frac{3}{40a^2} + \frac{1}{20a^2}\right) \cdot (C + ln\,2\,a) + e^{8a}E_i^2(-8a) \times \right.$$
$$\times \left(\frac{3}{40a^2} + \frac{11}{20a} + \frac{7}{5} + \frac{8a}{15}\right) + e^{4a}E_i^2(-8a)\frac{4a^2}{15} +$$
$$\left. + e^{4a}E_i^2(-4a)\left(-\frac{3}{20a^2} + \frac{1}{2a} - \frac{1}{5}\right) + \frac{1}{8a} - \frac{1}{10}\right]. \quad (10)$$

We will consider elementary chemical reactions as interactions between chemical bonds with positive and negative charges, i.e., we will consider these charges as the influence of a third Coulomb center on a separately selected chemical bond. In this case, the third Coulomb center causes some disturbance that acts on the chemical bond. Then we will present the Hamiltonian of a three-center system in the form [9, 11, 12]:

$$H_0 = -\frac{h^2}{2M_1}\Delta\vec{R}_1 - \frac{h^2}{2M_2}\Delta\vec{R}_2 - \frac{h^2}{2M_3}\Delta\vec{R}_3 + \frac{Z_1Z_2}{|\vec{R}_2 - \vec{R}_1|} + \frac{Z_1Z_3}{|\vec{R}_3 - \vec{R}_1|} + \frac{Z_3Z_2}{|\vec{R}_3 - \vec{R}_2|}, \quad (11)$$

where H_0 – Hamiltonian of the interaction of three particles. Let us introduce Jacobi coordinates:

$$\vec{R} = \frac{M_1\vec{R}_1 + M_2\vec{R}_2 + M_3\vec{R}_3}{M_1 + M_2 + M_3},\ r = R_3 - \frac{M_1\vec{R}_1 + M_2\vec{R}_2}{M_1 + M_2},$$
$$\vec{R} = \vec{R}_2 - \vec{R}_1,$$
$$H_0 = -\frac{\square^2}{2M_t}\Delta\vec{R} - \frac{\square^2}{2M}\Delta\vec{R} - \frac{\square^2}{2M}\Delta\vec{r} + \frac{Z_1Z_2}{R} + \frac{Z_1Z_3}{r_1} + \frac{Z_2Z_3}{r_2}, \quad (12)$$

where the symbols are introduced:

$$M_t = M_1 + M_2 + M_3, \quad \frac{1}{M} = \frac{1}{M_1} + \frac{1}{M_2}.$$

Taking these assumptions into account, let us consider two Coulomb centers as a basis, and represent the perturbation caused by the influence of the third center in the state $s = \frac{1}{2}, 0,0$ in the form of a Neumann expansion [15]:

$$W_3 = \frac{2Z_3}{R}\sum_{p=0}^{\infty}\sum_{m=-p}^{p}(-1)^m(2p+1)\left[\frac{(p-|m|)!}{(p+|m|)!}\right] \times$$
$$\times P_p^{|m|}(\lambda_<)Q_p^{|m|}(\lambda_>)P_p^{|m|}(\mu_3)Q_p^{|m|}(\mu_3)\,e^{im(\phi-\phi_3)}, \quad (13)$$

where $\lambda_3 = \frac{R_2+R_3}{R_1}$; $\mu_3 = \frac{R_2-R_3}{R_1}$; $R_1 = R$; R_2 – distance from atom 1 to atom 3; R_3 – distance from atom 2 to atom 3; $\lambda_{\lessgtr}$ – greater or less than the values; $P_p^{|m|}(\lambda_<)$ and $Q_p^{|m|}(\lambda_>)$ are the attached Legendre functions of the first and second kind. Then, taking into account the perturbation, the energy of the three-particle problem will be:

$$W_3 = \frac{\left\langle \Psi \left| H + W_{\frac{1}{2},0,0} \right| \Psi^* \right\rangle}{\langle \Psi | \Psi^* \rangle} = E_0(R_1) + \sum_{i=1}^{N}\frac{4aZ_i}{R_i\left[\frac{1}{2a} - \frac{4a}{3}e^{4a}E_i(-4a)\right]}\left\{Q_0^0(\lambda_3)\left[\frac{2}{3}e^{4a}E_i(-4a) - \frac{1}{4a^2}\right] - \right.$$
$$- \frac{1}{8a^2e^{2a(\lambda_3-1)}}[P_2(\lambda_3)P_2(\mu_3) - 1]\left[e^{2a(\lambda_3+1)}E_i(-2a(\lambda_3+1) - e^{2a(\lambda_3-1)}E_i(-2a(\lambda_3-1))\right] - Q_2(\lambda_3)P(\mu_3) \times$$
$$\times \left[\frac{2}{3}e^{4a}E_i(-4a) + (\lambda_3^2 - 1)e^{2a(\lambda_3-1)}E_i(-2a(\lambda_3-1)) + e^{-2a(\lambda_3-1)}\left(\frac{1}{2a} - \frac{1}{4a^2} - \frac{\lambda_3}{2a}\right) + \frac{1}{4a^2}\right] +$$
$$+ Q_0(\lambda_3)P_2(\lambda_3)P_2(\mu_3)\left[(\lambda_3^2 - 1)e^{2a(\lambda_3+1)}E_i(-2a(\lambda_3+1)) - \left(\frac{1}{2a} - \frac{1}{4a^2} - \frac{\lambda_3}{2a}\right)\right]e^{-2a(\lambda_3-1)} \cdot P_2(\lambda_3)P_2(\mu_3) \times$$
$$\left. \times \left[e^{4a}E_i(\lambda_3+1)E_i(-2a(\lambda_3+1)) + \frac{1}{2a}e^{-2a(\lambda_3-1)}\right]\right\}. \quad (14)$$

In the above expressions, $a = -1 + \sqrt{0.5 + Z^+ + [2(R_1R_2^2 - R_1^2R_2) + R_1^2R_2^2]\frac{\gamma R_2}{4R_1R_2}}$.

For identical atoms ($R_1 = R_2$), the last expression (14) reduces to $a = -1 + \sqrt{0.5 + Z^+ + \frac{\gamma R_2}{4}}$, where γ – frequency of the main oscillations of atoms), and in the absence of oscillations; $a = -1 + \sqrt{0.5 + Z^+}$. That is, the problem reduces to solving a two-center problem.

Thus, there are two terms in formula (13): the binding energy of the Cr molecule with one of the elements B, C, Al, Si, and additives, which are the influence of the third (or several) Coulomb centers on the chemical bond of a given molecule.

Let us calculate the binding energy of chromium compounds with B, C, Al, and Si (Fig. 2) using formula (13).

The calculation of the bonding energy curves showed that in the ground state (s=1/2), the interatomic distance and bonding energy coincide with the experimental data (0.189 a.u.) with an accuracy of 2%.

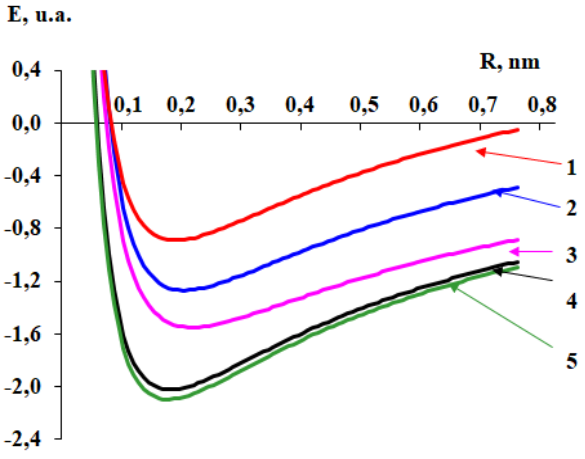

Fig. 2. Chemical bond energies of functional coatings: 1 – Cr-Cr; 2 – Cr-C; 3 – Cr-Al; 4 – Cr-Si; 5 – Cr-B

Using this method, we calculated the effect on the chemical bond of divalent atoms of the cubic structure of manganese, cobalt, iron, nickel, copper, and zinc,

which are located in the centers of tetrahedra and significantly affect octahedra with trivalent iron atoms, and thus also affect the chemical bond of oxygen [16, 17].

Calculation of chemical bond parameters for functional coatings

Chemical bond formula	Energy of chemical bond, a.u.	Interatomic distance of chemical bond R, nm
Cr-Cr	0.1486	0.2206
Cr-B	0.1982	0.1234
Cr-C	0.0793	0.1817
Cr-Si	0.1894	0.2183
Cr-Al	0.1181	0.2413

Quantum mechanical calculations showed that with an increase in the atomic number of the elements, the bond energy increases, and the interatomic distance O=O decreases, which corresponds to the experimental and tabulated values of the crystal lattice parameters (see Fig. 2, Table).

CONCLUSIONS

Summarizing the results of quantum mechanical modeling aimed at studying the energies of chemical bonds and interatomic distances in a number of compounds synthesized under conditions of non-stationary temperature influence, a number of fundamental conclusions can be drawn regarding the peculiarities of their structure formation. It has been shown that the non-equilibrium processes characteristic of such coating formation modes determine the intensive emergence of a wide range of phases and compounds that enrich functionally active systems and give them increased structural complexity. It has been established that the energy of chemical interactions directly depends on the individual characteristics of elements, in particular aluminum, boron, carbon, and silicon, which make a significant contribution to the formation of the final properties of materials. The patterns of chemical structure formation in environments with non-stationary temperature conditions open up the possibility of reliable prediction of conditions for the synthesis of fundamentally new types of compounds, as well as the creation of materials with a unique set of physicochemical characteristics, which broadens the prospects for their practical application. In addition, the proposed method of quantum-mechanical calculations has proven its versatility and can be used as a tool for determining bond energies in a much wider range of chemical systems, which makes it promising for further research and applied developments in the field of materials science.

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КВАНТОВО-МЕХАНІЧНА МОДЕЛЬ ВЗАЄМОДІЇ ІОНІВ ЛЕГУЮЧИХ АТОМІВ ВИСОКОЧИСТИХ МЕТАЛІВ

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За допомогою квантово-механічної моделі взаємодії іонів легуючих атомів чистих металів із металевою підкладкою у виді ланцюгу N-фінітних центрів встановлено, що вони розміщені вздовж прямої. Це дозволяє встановити тенденцію утворення тих чи інших високочистих сполук у разі отримання захисних хромованих покриттів, що формуються за нестаціонарних температурних умов. Нерівноважні процеси, характерні для таких режимів формування покриттів, зумовлюють інтенсивне виникнення широкого спектра фаз та сполук, які збагачують функціонально активні системи та надають їм підвищеної структурної складності. Шляхом розв'язання рівняння Шредінгера для заряду, що рухається в полі ланцюгу з N-фінітними центрами, отримано вирази для розрахунку енергії хімічного зв'язку іонів легуючих атомів. Встановлено, що енергія хімічних взаємодій безпосередньо залежить від індивідуальних характеристик високочистих елементів, які вносять значний внесок у формування кінцевих властивостей матеріалів.