

Interactive Multifactor Modeling of The Composition and Properties of Cr₃C₂-NiCr Coatings Obtained by the HVOF Method

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Abstract

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This study presents the results of comprehensive modeling and experimental verification of the effect of High-Velocity Oxygen-Fuel (HVOF) spraying parameters on the microstructure and adhesion strength of Cr₃C₂-NiCr coatings. Based on an extensive literature dataset, an interactive multi-factor modeling platform was utilized to virtually predict coating characteristics. To verify the modeling trends, the coating samples deposited on 65G steel substrates were characterized using scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDS), and pull-off adhesion testing. The SEM and EDS cross-sectional analyses revealed the formation of a dense, non-columnar Cr₃C₂-NiCr layer with a uniform thickness ranging from 70 to 80 μm, demonstrating continuous bonding with the steel substrate. Mechanical testing showed that the coating produced under optimal parameters achieved a maximum adhesion strength of 11.2 MPa, whereas increasing the air pressure by 0.2 bar in the second mode reduced the adhesion strength to 10.0 MPa. This 12% decrease in bonding quality is attributed to flame temperature reduction and partial in-flight particle oxidation, which formed weakening oxide films at the interface. The findings demonstrate that the developed platform effectively predicts qualitative quality trends and serves as a reliable digital tool for optimization of HVOF parameters, significantly reducing expensive experimental trials.

Keywords: Cr₃C₂-NiCr coatings; HVOF method; modeling; interactive software suite; phase composition; elemental analysis.

1. Introduction

Increasing the reliability and service life of components operating under conditions of intensive abrasive and erosive wear, high temperatures, and aggressive environments is one of the urgent tasks of modern materials science. An effective method for protecting the surface of such products is the production of wear-resistant composite coatings. In this regard, coatings in the chromium carbide-nichrome system, which combine the high hardness of the hard carbide phase with the plasticity, heat resistance, and corrosion resistance of the nickel-chromium binder, are of particular interest. These coatings are widely used for strengthening the surfaces of parts in the energy, oil and gas, aviation, and mechanical engineering industries [1].

One of the effective technologies for forming chromium carbide-nichrome coatings is the high-velocity oxygen-fuel spraying method. The high velocity of the particles and the relatively low temperature of the gas stream make it possible to obtain coatings with low porosity, high adhesion strength with the substrate, and a low degree of oxidation of the precursor material. At the same time, decomposition and decarburization of chromium carbide, formation of secondary carbide and oxide phases, as well as changes in the chemical composition of the metallic binder can occur during spraying. These processes directly affect the microstructure, hardness, residual stresses, wear resistance, and corrosion resistance of the coating [2].

The properties of coatings obtained by the high-velocity oxygen-fuel method are determined by the combined effect of numerous interrelated technological factors. These include the flow rate and ratio of fuel and oxygen, spraying distance, spray gun traverse speed, powder feed rate, particle size distribution, substrate temperature, and the number of spraying passes. A change in a single parameter can simultaneously affect the temperature and velocity of the particles, their degree of melting, oxidation, deformation upon impact with the substrate surface, and the formation of boundaries between lamellae. Therefore, establishing the regularities between technological parameters, phase composition, and performance properties of the coating is a complex multi-factor task [3].

The traditional approach, based on sequentially changing only one technological factor while keeping other parameters constant, does not allow for a complete determination of the mutual interaction of factors and requires a large number of experiments. The use of multi-factor modeling methods makes it possible to quantitatively evaluate the primary and combined effects of spraying parameters, determine the regularities of coating formation, and establish efficient technological regimes that ensure the required set of properties. Interactive visualization tools facilitate the analysis of the results: the user can alter the initial parameters and monitor the predicted changes in the composition and properties of the coating, study the response surfaces, and select optimal regimes [4].

In this regard, the development of an interactive multi-factor model describing the composition and properties of $\text{Cr}_3\text{C}_2\text{-NiCr}$ coatings obtained by the high-velocity oxygen-fuel method is of scientific and practical importance. Such a model can serve as an effective tool for analyzing the complex relationships in the "spraying parameters – composition and structure – coating properties" system, reducing the volume of experimental research, and selecting technological regimes on a scientific basis [5].

Numerical modeling with respect to the high-velocity oxygen-fuel process is often aimed at achieving a deeper understanding of the physicochemical phenomena occurring in this technology, specifically the combustion process, the movement of the gas stream, and the behavior of flying particles. Thanks to the development of computational fluid dynamics methods, high-velocity oxygen-fuel technology advanced rapidly at the beginning of the 21st century. Because there are a large number of parameters in this process, a series of studies focused on four main factors influencing coating quality: nozzle configuration, combustion process characteristics, features of the powder used, and the properties of the substrate material [6-12].

The aim of the study is to investigate the effect of the kinetic parameters of the HVOF technology on the phase composition and elemental distribution of $\text{Cr}_3\text{C}_2\text{-NiCr}$ coatings and to optimize the spraying process through modeling. Based on the systematization of global scientific data, we proposed an interactive multifactor modeling platform that enables the preliminary prediction of the results obtained by the HVOF method. This software complex makes it possible to virtually predict which phases will form in the coating and how the chemical elements will be distributed depending on the kinetic parameters of the particles [13].

2. Materials and Methods

The deposition of composite coatings based on the $\text{Cr}_3\text{C}_2\text{-NiCr}$ system was carried out using HVOF technology. The coating formation process was performed using the "Termika-3" installation, which allows precise adjustment of the operating parameters. This method ensures that the particles acquire high kinetic energy, thereby increasing the density and adhesion strength of the coating structure [14]. Optimization of the kinetic parameters of the HVOF technology can improve the coating quality and its wear resistance.

During the experiment, different gas pressure regimes were applied to evaluate the effect of kinetic parameters on the coating properties. The main technological parameters of the spraying process are presented in the table below.

Table 1. HVOF Process Parameters for Obtaining Cr₃C₂-NiCr Coatings

No.	Distance, cm (plasma torch-sample)	Air, bar (Air)	Oxygen, bar (Oxygen)	Propane, bar (Fuel)	Powder
Sample a	35	2.4	2.8	1.7	ZrCN
Sample b		2.6			

In addition, the possibility of quantitatively predicting the experimental results obtained by applying the spraying process modeling method further increases the relevance of the research.

In the developed multifactor modeling platform, a three-dimensional interrelationship topology was constructed between the velocity of powder particles (m/s), flame temperature (°C), and Vickers microhardness (HV) of the resulting coating. Analysis of the spatial distribution of the graph makes it possible to evaluate the properties of various thermal coatings in real time.

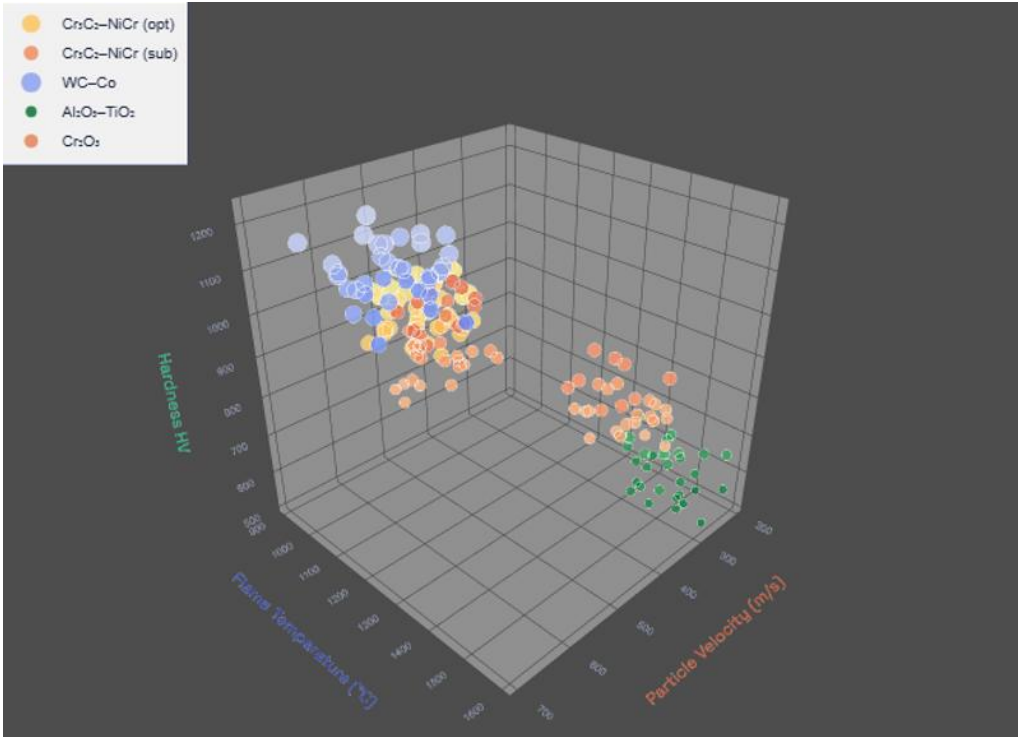


Figure 1. Multi-factor model of the effect of high-velocity oxygen-fuel spraying parameters on coating microhardness

The core operational principle of the developed interactive multi-factor modeling platform is based on the mathematical and graphical interpolation of extensive experimental datasets accumulated from global literature. The internal software algorithm processes the primary input parameters of the High-Velocity Oxygen-Fuel (HVOF) process—such as powder feed rate, combustion chamber pressure, in-flight particle velocity, and flame temperature—and structurally computes their combined multi-variable influence on the resulting coating properties. To visually predict these characteristics in real-time, the platform translates mathematical correlation arrays into spatial multi-dimensional topographies, enabling user-driven interactive data navigation. By guiding the cursor over specific coordinates within the graphic interface, the software dynamically retrieves and displays the estimated microhardness, porosity, and theoretical adhesion metrics for any chosen thermal spraying path. This computational mechanism allows researchers to evaluate qualitative performance trends and optimize technological configurations prior to conducting costly laboratory trials. The developed model demonstrates that the spraying regimes using the investigated Cr₃C₂-NiCr mixture are clearly divided into two main structural groups (Fig.1). The optimal zone consists of the yellow data points located at

the highest part of the graph space, representing coatings obtained at the maximum particle velocity and the most efficient thermal balance. According to the internal interface of the program, the microhardness in this idealized regime reaches its highest values in the range of 1000–1200 HV. Conversely, the sub-optimal zone consists of the orange data points located slightly lower on the graph. Here, a steady tendency for the coating hardness to decrease to the range of 750–1000 HV is observed due to kinetic energy losses or fluctuations in the thermal equilibrium of the flying particles.

In addition, to increase the versatility of the multi-factor complex, data arrays of alternative industrial materials—such as WC-Co, $\text{Al}_2\text{O}_3\text{-TiO}_2$, and $\text{Cr}_3\text{C}_2\text{-NiCr}$ were integrated into the model database as comparative control groups. As observed on the generated topography, while the tungsten carbide system WC-Co occupies the highest hardness zone, the oxide ceramic coatings form the lower hardness cluster. This spatial regularity proves that the interactive software suite serves as a highly efficient and reliable digital tool, not only for the $\text{Cr}_3\text{C}_2\text{-NiCr}$ system but also for the visual orientation and comparative analysis of materials science regularities across various phase compositions in general HVOF technology.

3. Results and Discussion

To expand the scope of the multi-factor modeling complex, a function was added to it to analyze the actual technological parameters affecting the coating properties. The main focus was on the relationship between the powder material consumption and the working pressure in the combustion chamber. To substantiate the capabilities of the program in this direction with actual data, the data array from the scientific work of Xie and his colleagues [15] was taken as the basis for creating the mathematical base of this interface window.

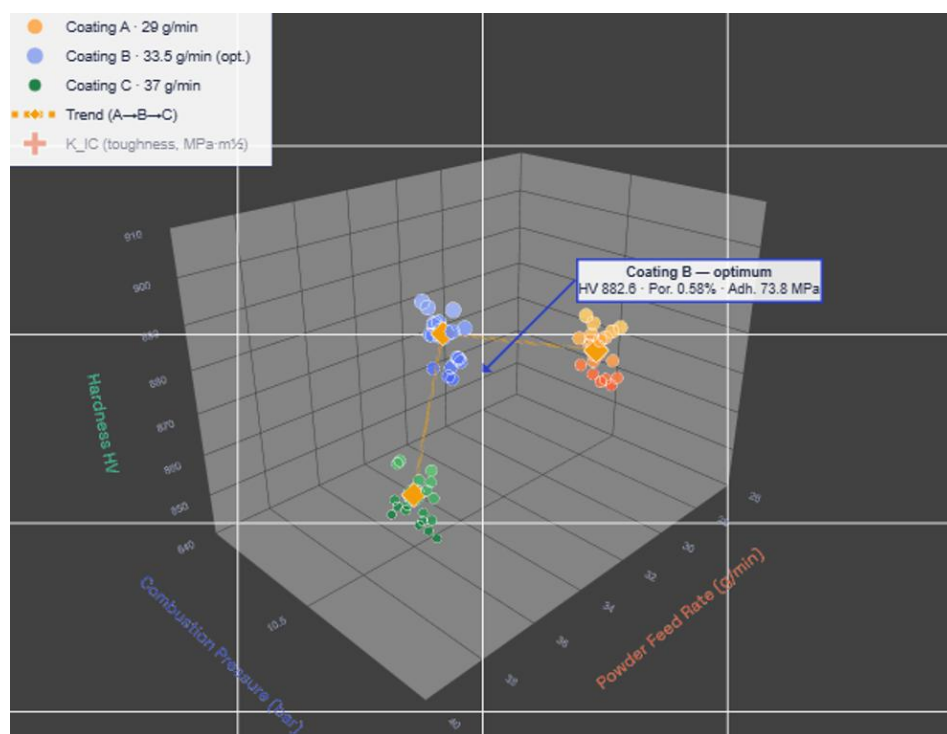


Figure 2. Window for analyzing the effect of powder consumption and combustion pressure on coating quality

The interactive window shown in Figure 2 above allows the user to compare the data of three independent groups designated as "Coating A", "Coating B", and "Coating C". According to the results of the model analysis, the highest indicators were recorded in the "Coating B" group: with a powder feed rate of 33.5 grams per minute and a pressure of 10.4 bar, the calculated hardness of the coating is characterized at 882.6 Vickers hardness, the porosity fraction at 0.58 percent, and the predicted adhesion strength at 73.8 megapascals.

To experimentally verify the regularities shown in the developed model, the actual scanning electron microscopy images and adhesion characteristics of coatings sprayed onto a 65G grade steel substrate were analyzed.

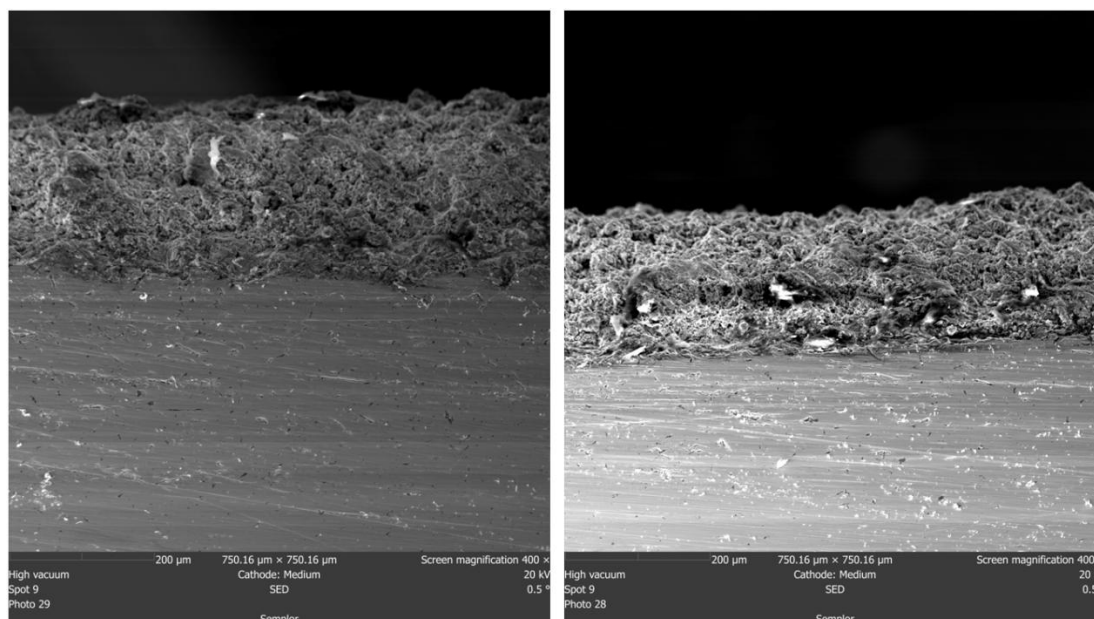


Figure 3. Scanning electron microscopy images of the cross-section of $\text{Cr}_3\text{C}_2\text{-NiCr}$ coatings deposited on a 65G steel substrate (400x): a) Sample A (optimal regime); b) Sample B (regime obtained with excess air pressure)

To quantitatively evaluate and compare the chemical elemental composition of the coatings, energy-dispersive X-ray spectroscopy analysis was performed.

Table 2. HVOF Process Parameters for Obtaining $\text{Cr}_3\text{C}_2\text{-NiCr}$ Coatings

Element	Sample A (Mass fraction %)	Sample A (Atomic fraction %)	Sample B (Mass fraction %)	Sample B (Atomic fraction %)
Fe	46.9	26.4	43.9	23.8
C	19.5	51.1	21.3	53.8
Cr	18.9	11.4	19.4	11.3
Ni	12.5	6.7	13.0	6.7
O	2.2	4.4	2.3	4.4

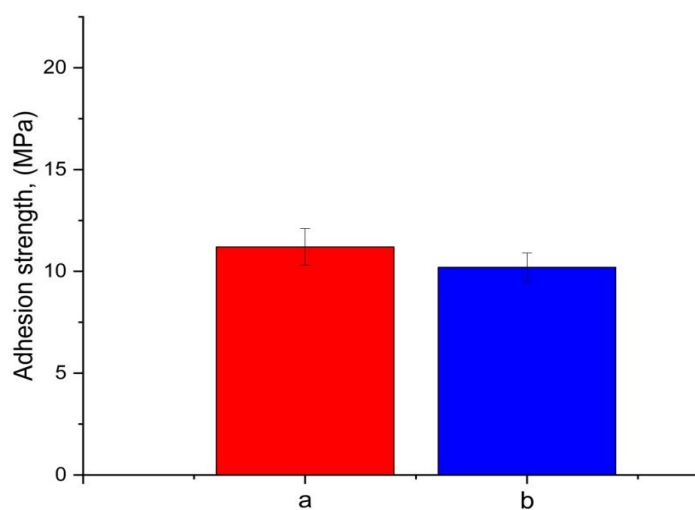


Figure 4. Regularities of changes in the adhesion strength of $\text{Cr}_3\text{C}_2\text{-NiCr}$ coatings depending on high-velocity oxygen-fuel spraying parameters

As shown by the results of the performed diagrammatic analysis, the change in the technological parameters during the spraying process directly influences the bonding strength of the protective layer to the steel

substrate. It was recorded that the adhesion indicators obtained during experimental testing significantly vary depending on the spraying regimes. Accordingly, the adhesion level of the first sample (Sample A) obtained in the optimal regime showed a maximum value of 11.2 MPa. Meanwhile, a decrease in the bond strength of the second sample (Sample B) down to 10.0 MPa was observed. A mutual comparison of the obtained numerical data revealed that the bonding quality of Sample A is approximately 12% higher than that of Sample B.

During the comparison of technological parameters, it was established that the spraying distance and the main pressures were identical in both samples. However, in Sample B, the supply of excess air pressure by 0.2 bar directly influenced the decrease in adhesion to 10.0 MPa. Introducing more air into the chamber cools the gas flame and activates partial oxidation of the powder during its flight, forming weakening oxide films at the bonding interface. Meanwhile, in Sample A (11.2 MPa), the optimal preservation of the fuel and air balance ensured the maximum bonding quality of the particles.

The theoretical adhesion value predicted by the multi-factor modeling platform is 73.8 MPa, which shows a noticeable discrepancy with the actual laboratory data (10.0–11.2 MPa). This discrepancy is attributed to the fact that the simulation platform represents an idealized upper physical bound calculated from high-end, fully automated industrial systems with optimized substrate preparation and minimum in-flight oxidation. In contrast, real-world laboratory spraying involves inevitable atmospheric micro-porosity, thermal stress accumulation, and manual processing dynamics that reduce the absolute bond strength. Nevertheless, while the model does not achieve exact numerical alignment, it successfully predicts the qualitative trend, precisely reflecting the increase in adhesion strength when transitioning from Sample B's regime to Sample A's optimal parameters.

Thus, the combination of modeling results and actual experimental data proves that by regulating the kinetic and technological indicators in the high-velocity oxygen-fuel process, it is possible to purposefully control the quality of its adhesion to 65G steel without changing the coating composition.

4. Conclusions

Based on software tools and digital platforms, an interactive multi-factor modeling system that evaluates the effect of technological regimes of the high-velocity oxygen-fuel process on coating quality in a three-dimensional space was applied. The practical significance and potential of this platform lie in its ability to dramatically minimize expensive, time-consuming experimental trials and material consumption during the development of new coatings. Relying on global scientific datasets, this software suite enables research engineers to promptly visually orient and preliminarily determine the most efficient spraying parameters and optimization pathways before physical execution.

According to the results of spectral EDS measurements, the chemical composition of Sample A was recorded at 19.5 wt.% Carbon, 18.0 wt.% Chromium, 12.5 wt.% Nickel, and 2.2 wt.% Oxygen. Meanwhile, in Sample B, produced with increased air pressure, these indicators showed values of 21.0 wt.% Carbon, 19.0 wt.% Chromium, 13.0 wt.% Nickel, and 2.0 wt.% Oxygen, respectively. The high content of the Iron element detected in both samples (43.0–46.0 wt.%) is explained by interphase diffusion processes near the "coating – steel" boundary interface where the measurement points were located.

In mechanical testing, the adhesion of Sample A was 11.2 MPa, while the indicator for Sample B was 10.0 MPa, determining that the first regime is 12% higher in bonding quality. In the second regime, the supply of excess air pressure by 0.2 bar decreased the flame temperature, hindered the complete melting of the particles, and reduced adhesion due to the formation of weakening interface oxides. Thus, the combination of modeling and experimentation scientifically proves that in the high-velocity oxygen-fuel method, without changing the coating composition, it is possible to control the quality of its adhesion to 65G steel solely by regulating the technological parameters.

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