Computer-aided simulation of WC-10Co-4Cr cermet coatings formation and predictive detection of optimal spraying regimes

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Abstract. The results of computational experiments on the formation of thermal spray WC-10Co4Cr coatings are presented. The effect of sprayed particles velocity (200-1000 m/s), temperature (1600-2500 K) and the size (15-40 microns), as well as substrate temperature (300-600 K), on the properties of coatings (porosity, roughness, adhesion) has been studied. Ranges of particle parameters have been determined, which ensure their spreading process without «splashing» and the formation of coatings with low porosity and high adhesion. A qualitative comparison of the calculation results with experimental data on high-velocity plasma spraying of WC-10Co4Cr coatings is carried out.

1. Introduction
Tungsten carbide coatings with cobalt and chromium additives (WC/Co-Cr) are widely used in various industries, including aviation, mining and automotive, to protect against wear and corrosion. For example, these coatings were applied to aircraft shafts and landing gear because of their high hardness and excellent erosion and abrasion resistance (instead of the commonly used chromium plating, [1]).

For example, tungsten carbide with cobalt and chromium, corresponding to the composition WC-14wt%CoCr (metal bond corresponds to the composition 10 wt %Co-4wt.%Cr), is resistant to erosion and abrasion, recommended for aqueous solutions. The Co-Cr matrix gives high resistance to abrasion and corrosion in comparison with materials of various WC-Co compositions. Composition WC-14wt%CoCr is used to protect against wear on rollers in the paper industry, in wet corrosion conditions. Its oxidation resistance is up to 650 °C [2].

It is known from the coating technology [2] that the tendency to form cracks greatly increases with increasing layer thickness, since, in essence, the sprayed coating has a layered structure with pores consisting of many highly plastic microplates - splats. This risk, first of all, takes place for hard coatings, for example, with a strong difference in behavior during thermal expansion of the coating materials and the base. If it is nevertheless necessary to apply a thick coating, then intermediate layers are used that provide adhesion and stress equalization.

Corrosion resistance of sprayed coatings is mainly determined by applying coatings from many corrosion-resistant materials. However, it must be borne in mind that when spraying, the alloy composition changes as well. So, for example, for stainless and acid-resistant steels, depletion of...
chromium can occur at the edges of microplates, then after spraying these materials can only conditionally serve as protection against corrosion and acids. If pure elements such as nickel or chromium are sprayed, no change is observed. Ceramic materials are particularly corrosion resistant. During thermal spraying, the decomposition of WC particles occurs. Intensive decomposition or decarburization of WC particles can be caused by excessive temperatures during their application, which leads to the formation of several phases, such as $\text{W}_2\text{C}$, $\eta\cdot\text{Co}_x\text{W}_y\text{C}_z$ ($\text{Co}_6\text{W}_6\text{C}$ and $\text{Co}_3\text{W}_3\text{C}$), dissolution of tungsten metal and carbon in the binder phase, as well as the formation of an amorphous Co phase due to rapid solidification upon impact. However, not only the thermal spraying system [1] depends on the microstructure and characteristics of WC/Co-Cr coatings, but also largely on the particles of the powder of the feedstock material (type, morphology, composition) and spraying parameters. In addition, tungsten carbide coatings have a wide range of properties and microstructural features depending on the phase content, powder and carbide particle size, carbide particle distribution, porosity and cohesion of WC particles with CoCr matrix [1].

Therefore, when such coatings are produced with thermal spraying methods (plasma, detonation, HVOF, etc.), an important aspect is the study of ways to control the phase composition and microstructure of the coatings, the determination of the coating spraying regimes with optimal functional characteristics. Conducting a large cycle of physical experiments to achieve this goal is associated with large material, financial and time costs. In this regard, computer simulation of the formation of a coating during its deposition by gas thermal methods, followed by an assessment of the basic functional characteristics of the coatings, which allows predicting optimal spraying conditions, is an effective research approach.

2. Methodological aspects of computer simulation of coatings
To carry out a large number of computational experiments (CE) at the stage of computer simulation of the layered structure of coatings and predict their functional characteristics, the program system «parallel execution of the SIMD-task cycle» [3] was used, which makes it possible to significantly speed up the execution of entire CE cycle due to the simultaneous parallel execution of similar tasks (figure 1).

![Diagram](image-url)

**Figure.** 1. Structure of a program system.
The same single instruction (SI) is executed on all computing nodes (CN), simulating the process of coating formation on each CN with a certain set of initial data (a set of initial «key physical parameters», KPPs) of sprayed powder particles and substrate. The sets of KPPs loaded on all CNs differ from each other and form multi data (MD) blocks. The program system (figure 1) manages the process of downloading program codes and data blocks to a control unit, synchronizes and monitors parallel computing processes, and also controls the upload of calculation results from all control units to a common storage in the form of a database (DB) on an external drive. In addition, the program system presents the results of calculations in a convenient form for analysis - electronic report containing tables, graphs, figures, etc.

In study [8], the results of computer simulation of cermet coatings TiC-30vol.%NiCr and their functional characteristics using the program system «parallel execution of the SIMD-task cycle», which are in good agreement with experimental data, are presented. In this work, we continue the experience gained in computer simulation of cermet coatings of a different composition based on tungsten carbides in conjunction with the CoCr metal alloy.

In computational experiments (CE) for simulation WC-10Co-4Cr cermet coatings, a 2x2 mm plate made of grade 45 steel was used as a substrate. Taking into account the ratio of the mass fractions of tungsten carbide (86%) and CoCr metal binder (14%) using program system, the thermophysical properties of WC-10Co-4Cr cermet particles (as well as density, dynamic viscosity, etc.) used to model the layered structure of the corresponding coatings were calculated.

At the simulation stage of WC-10Co-4Cr cermet coatings, four sets of parametric calculations were performed (tables 1-4) both of the splat parameters \(D_s, \overline{D_s}, h_s\) and for the functional characteristics of the coatings \(P, R_s, \bar{\sigma}_{add}\).

In the first set of calculations, when the particle temperature \(T_p\) changes in the range from 1600 to 2500 K (in increments of 100 K), the following values of the particle KPP were kept constant (table 1): particle diameter \(D_p = 35 \, \mu m\), particle velocity \(U_p = 700 \, m/s\), the temperature of the steel substrate \(T_b = 400 \, K\).

In the second cycle of calculations, when the particle velocity \(U_p\) was varied in the range from 200 to 1000 m/s (in increments of 100 m/s), the following values of the particle KPP were kept constant (table 2): particle temperature \(T_p = 1600 \, K\), particle diameter \(D_p = 35 \, \mu m\), the temperature of the steel substrate \(T_b = 400 \, K\).

In the third set of calculations, when the particle diameter \(D_p\) was varied in the range from 15 to 40 \(\mu m\) (in increments of 5 \(\mu m\)), the following values of the particle KPP were kept constant (table 3): particle temperature \(T_p = 1600 \, K\), particle velocity \(U_p = 700 \, m/s\), the temperature of the steel substrate \(T_b = 400 \, K\).

In the fourth set of calculations, when the temperature of the substrate (base) \(T_b\) in the range from 300 to 600 K (in increments of 100 K) was changed, the following values of the particle KPPs were kept constant (table 4): particle temperature \(T_p = 1600 \, K\), particle velocity \(U_p = 700 \, m/s\), the particle diameter \(D_p = 35 \, \mu m\).

In Tables 1-4, in addition to the value of the splat diameter \(D_s\) (microns), there is a normalized value of the splat diameter \(\overline{D_s} = D_s / D_p\) (r.u.) and which is also called the «spreading factor» of the melt particle. Along with the splat thickness \(h_s\), a normalized thickness value \(\overline{h_s} = h_s / D_p\) is also given. \(P\) is the coating porosity, and \(R_s\) is the surface roughness of the coating. The value \(\bar{\sigma}_{add}\) is the relative adhesive strength of the first monolayer of the coating to the substrate, in other words, the ratio of the absolute adhesive strength of the coating to the material tensile strength, i.e. fraction of the maximum possible adhesive strength. The value of \(T_c\) shows the contact temperature at the point of impact of the melt particle with the surface (in the first coating layer with the substrate, and in the next layers with the sprayed layer of the same WC-10Co-4Cr particles). In addition, a transition from the 1st scenario of the formation of the splat to the 3rd is possible (table 1).
3. Analysis of the computational experiments (CEs) results

The results of CEs simulation coatings (200 μm thick) are summarized in tables 1–4, in which, in addition to the characteristics of the coatings, the corresponding KPPs of the powder particles and the calculated parameters of the splats are given.

**Table 1.** The calculated parameters of the splats and the functional characteristics of the coatings with a change in the particle temperature parameter $T_p$ taking into account the conditions: $U_p = 700$ m/s, $D_p = 35$ μm, $T_b = 400$ K.

| $T_p$ K | $D_s$ μm | $D_{s, r.u.}$ | $h_s$ μm | $h_{s, r.u.}$ | $P$, % | $R_s$ μm | $\sigma_{adg}$, r.u. | $T_c$, K | Scenario |
|---------|-----------|----------------|------------|---------------|-------|-------------|-----------------|----------|----------|
| 1600    | 106       | 3.032          | 2.54       | 0.073         | 0.16080 | 2.982       | 0.3085          | 919.8    | 1        |
| 1700    | 119       | 3.391          | 2.03       | 0.058         | 0.12654 | 2.460       | 0.2751          | 988.5    | 1        |
| 1800    | 135       | 3.862          | 1.56       | 0.045         | 0.03493 | 2.199       | 0.2080          | 1068.0   | 1        |
| 1900    | 218       | 6.239          | 0.60       | 0.017         | 0.00178 | 3.640       | 0.6335          | 1624.7   | 3        |
| 2000    | 218       | 6.239          | 0.60       | 0.017         | 0.00011 | 3.807       | 0.8621          | 1706.3   | 3        |
| 2100    | 218       | 6.239          | 0.60       | 0.017         | 0.00024 | 3.814       | 0.9937          | 1869.6   | 3        |
| 2200    | 218       | 6.239          | 0.60       | 0.017         | 0.00013 | 4.102       | 0.9996          | 1951.3   | 3        |
| 2300    | 218       | 6.239          | 0.60       | 0.017         | 0.00008 | 3.974       | 0.9999          | 2032.9   | 3        |
| 2400    | 218       | 6.239          | 0.60       | 0.017         | 0.00013 | 3.892       | 1.0000          | 2114.6   | 3        |
| 2500    | 218       | 6.239          | 0.60       | 0.017         | 0.00013 | 3.892       | 1.0000          | 2114.6   | 3        |

**Table 2.** Calculated parameters of the splats and the functional characteristics of the coatings with a change in the particle velocity parameter $U_p$ taking into account the conditions: $T_p = 1600$ K, $D_p = 35$ μm, $T_b = 400$ K.

| $U_p$, m/s | $D_s$ μm | $D_{s, r.u.}$ | $h_s$ μm | $h_{s, r.u.}$ | $P$, % | $R_s$ μm | $\sigma_{adg}$, r.u. | $T_c$, K | Scenario |
|-------------|-----------|----------------|------------|---------------|-------|-------------|-----------------|----------|----------|
| 200         | 79        | 2.253          | 4.59       | 0.131         | 6.2845 | 4.218       | 0.2415          | 919.8    | 1        |
| 300         | 87        | 2.478          | 3.80       | 0.109         | 4.3492 | 3.741       | 0.2834          | 919.8    | 1        |
| 400         | 93        | 2.652          | 3.32       | 0.095         | 1.8556 | 3.440       | 0.3065          | 919.8    | 1        |
| 500         | 98        | 2.797          | 2.98       | 0.085         | 0.6516 | 3.259       | 0.3063          | 919.8    | 1        |
| 600         | 102       | 2.922          | 2.73       | 0.078         | 0.2798 | 3.001       | 0.2684          | 919.8    | 1        |
| 700         | 106       | 3.032          | 2.54       | 0.073         | 0.1608 | 2.982       | 0.3085          | 919.8    | 1        |
| 800         | 110       | 3.131          | 2.38       | 0.068         | 0.0440 | 2.525       | 0.2759          | 919.8    | 1        |
| 900         | 113       | 3.222          | 2.25       | 0.064         | 0.0023 | 2.825       | 0.3046          | 919.8    | 1        |
| 1000        | 116       | 3.305          | 2.14       | 0.061         | 0.0003 | 2.878       | 0.2526          | 919.8    | 1        |

**Table 3.** Calculated parameters of the splats and the functional characteristics of the coatings when changing the particle diameter parameter $D_p$ taking into account the conditions: $T_p = 1600$ K, $U_p = 700$ m/s, $T_b = 400$ K.

| $D_p$, μm | $D_s$ μm | $D_{s, r.u.}$ | $h_s$ μm | $h_{s, r.u.}$ | $P$, % | $R_s$ μm | $\sigma_{adg}$, r.u. | $T_c$, K | Scenario |
|-----------|-----------|----------------|------------|---------------|-------|-------------|-----------------|----------|----------|
| 15        | 37        | 2.478          | 1.63       | 0.109         | 0.038 | 2.509       | 0.3113          | 919.9    | 1        |
| 20        | 53        | 2.652          | 1.90       | 0.095         | 0.060 | 2.804       | 0.3202          | 919.9    | 1        |
| 25        | 70        | 2.797          | 2.13       | 0.085         | 0.100 | 2.746       | 0.2729          | 919.9    | 1        |
| 30        | 88        | 2.922          | 2.34       | 0.078         | 0.134 | 2.701       | 0.2777          | 919.9    | 1        |
| 35        | 106       | 3.032          | 2.54       | 0.073         | 0.160 | 2.982       | 0.3085          | 919.9    | 1        |
| 40        | 125       | 3.131          | 2.72       | 0.068         | 0.185 | 2.873       | 0.2966          | 919.9    | 1        |
The spreading factor for metal splats [9] should not exceed 4.5, and for ceramic and cermet splats [10] it should not exceed 5 (otherwise, the integrity of the splat form is not guaranteed). As can be seen from table 1, particle temperatures $T_p$ in excess of 1800 K are not acceptable during spraying, since in this case the spreading factor exceeds the permissible value of 5 (in this case, the spreading scenario changes).

Tables 1 and 2 confirm the fact that with increasing particle velocity and temperature, the porosity decreases, and with increasing particle diameter (table 3), the porosity increases (slowing down the growth rate). With a change in the substrate temperature $T_s$ in the range from 300 to 500 K (table 4), the porosity practically does not change (with a further increase in $T_s$, the expected slight decrease is observed).

The roughness of the sprayed surface with increasing particle temperature (to an acceptable value of 1800 K, table 1), as well as with an increase in the particle velocity (table 2), tends to decrease, since the thickness of the splats also decreases. With an increase in the particle diameter, a slight increase in the thickness of the splats is observed; therefore, the roughness of the coatings also increases slightly. With an increase in the temperature of the substrate (table 4), the thickness of the splats decreases, and therefore, the roughness of the coatings decreases.

It is known [11] that with an increase in the particle temperature and, consequently, with an increase in the contact temperature $T_c$, the relative adhesive strength $\bar{\sigma}_{adg}$ at first substantially increases, and at the end of the temperature range, the growth slows down and $\bar{\sigma}_{adg}$ asymptotically approaches 1. The adhesion strength of the first monolayer of splats on the substrate is mainly determined by the liquid phase of the CoCr alloy. Therefore, when calculating the adhesive strength of the first monolayer of splats with a substrate, the properties of the CoCr alloy were taken into account. Table 1 confirms the above growth trend of $\bar{\sigma}_{adg}$. The contact temperature $T_c$, as can be seen from table 4, does not change significantly, therefore, the adhesive strength $\bar{\sigma}_{adg}$ practically does not change. Following the theoretical concepts [11], the adhesive strength does not change with a change in the particle velocity, which is confirmed by table 2.

In [12], for the WC – Co coating with the MoS$_2$ composition, the absolute value of the adhesive strength of the coating is of the order of 132 MPa. In another work [13], an average adhesion value of the order of 250 MPa was indicated for the WC-12Co coating, and the experimental values of adhesion range from 210 to 280 MPa. For the CoCr alloy manufactured by Degudent [14], which is close in composition to the 10Co-4Cr alloy used in this work, the value of tensile strength 850 MPa is indicated. If the absolute value of 850 MPa, equal to the tensile strength, is multiplied by the value of the relative adhesive strength $\bar{\sigma}_{adg}$, taken from tables 1-4 as corresponding to the optimal spraying mode and equal to approximately 0.3, then the absolute value of the adhesive strength of the WC-10Co-4Cr coating is estimated at 255 MPa, which correlates well with the value given in [13].

In figure 2 the results of the study of WC-10Co-4Cr coatings produced by the high-velocity (supersonic) atmospheric plasma spraying [15] are shown. In experiments, a powder of 15-38 µm in size was sprayed. The use of optical diagnostics [16, 17] made it possible to establish that the average particle temperature was 2447 K and the average velocity was 412 m/s (figures 2a and 2b). Figure 2c

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**Table 4.** Calculated parameters of the splats and the functional characteristics of the coatings when changing the substrate temperature parameter $T_s$ taking into account the conditions: $T_p = 1600$ K, $U_p = 700$ m/s, $D_p = 35$ µm.

| $T_s$, K | $D_i$, µm | $\bar{D}_S$, r.u. | $h_i$, µm | $\bar{h}_S$, r.u. | $P$, % | $R_i$, µm | $\bar{\sigma}_{adg}$, r.u. | $T_s$, K | Scenario |
|---------|----------|------------------|---------|------------------|-------|----------|------------------|---------|---------|
| 300     | 104      | 2.958            | 2.67    | 0.076            | 0.1605| 3.073    | 0.2770           | 846.9   | 1       |
| 400     | 106      | 3.032            | 2.54    | 0.073            | 0.1608| 2.982    | 0.3085           | 919.8   | 1       |
| 500     | 109      | 3.116            | 2.40    | 0.069            | 0.1618| 2.726    | 0.3047           | 991.6   | 1       |
| 600     | 112      | 3.212            | 2.26    | 0.065            | 0.1520| 2.589    | 0.2779           | 1062.2  | 1       |
shows a general view of a 180 μm thick coating cross-section. The measured roughness of the coating was $R_a = 5.1 \mu m$ (figure 2d), and the porosity was 0.08% (figure 2e). As table 2 shows, at a particle temperature of 1600 K, a particle velocity above $U_p = 500-700$ m/s provides a decrease in porosity to a level of less than 0.5%.

**Figure 2.** Experimental results on WC/10Co4Cr coating deposition using high-velocity APS system: a) particles temperature distribution, b) particles velocity distribution, c) WC/10Co4Cr coating crosscut, d) coating roughness analysis, e) coating porosity analysis.

Based on the results of the calculations in tables 1 and 2, it is clear that increasing the temperature of the particles allows obtaining dense coatings at lower particle velocities. These conclusions are consistent with the experimental results in figure 2: at a particle temperature of $T_p = 2400$ K, dense coatings form even at a velocity of about $U_p = 400$ m/s. In this case, attention should be paid to the signs of the layered structure of the coating (figure 2e), which may indicate the realization of scenario No. 3 during particle spreading.

**4. Conclusions**

Using the computational experiments the effect of key physical parameters (particles velocity 200-1000 m/s, temperature 1600-2500 K and the size 15-40 microns, substrate temperature 300-600 K) on the properties of coatings (porosity, roughness, adhesion) has been studied. For the stable formation of metal splats and coatings, taking into account the condition ($\bar{D}_S < 5$), as well as the minimum porosity and maximum adhesive strength, we can assume that the optimal plasma spraying mode is: particle velocity $U_p = 500$ m/s, particle temperature $T_p = 1600-1800$ K, particle diameter $D_p = (30 \pm 10)$ μm, $T_b = 400-500$ K. The obtained conclusions are consistent with the experimental results on WC-10Co-4Cr coatings deposition using high-velocity (supersonic) atmospheric plasma spraying.
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