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Computer experiment on studying the properties of thermally sprayed alumina coatings with lamellar structure

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Abstract. Results of stochastic modeling of lamellar structure formation and characteristics (microstructure, porosity, roughness) of ceramic coatings made of corundum powders (α-phase of Al_2O_3) are given in conditions typical for atmospheric plasma spraying (APS), and also detonation and supersonic flame spraying (HVOF). Comparison of characteristics of coatings for two model splats morphologies at their random laying on the base surface is presented.

Thermal spraying of coatings made of metal oxides powders (Al_2O_3, ZrO_2, TiO_2, Cr_2O_3, etc.) is widely used in industry for application of protective surface layers of various functionality. With that, increase in quality and improvement of structure of the sprayed materials in many ways depend on comprehension of the processes taking place at stochastic laying of splats as a result of which lamellar structure of coating is formed.

Despite the fact that a considerable amount of experimental data about the functional characteristics of thermally sprayed coatings is gathered so far, this data is insufficiently systematized. Thereof, there is no comprehensive approved idea of interrelation between spraying conditions and properties of sprayed coatings. In this regard, the computational technology, including program code, for modeling of lamellar structure formation of thermally sprayed coatings and their functional characteristics are presented in paper [1], which use, in our opinion, will promote more targeted design of the required coatings. Besides the problem-oriented core, the software includes several subsystems, in particular, the visualization subsystem of structure and surface morphology of coatings, and also the expandable referral database on properties of materials.

The “SPLAT” subsystem allows calculating geometrical characteristics of splats (melt droplets, spread and solidified on the base surface) at the preset values of key physical parameters (KPPs): particles velocity, temperature and size prior to impact, temperature of base and morphology of its surface. Besides, with the help of this subsystem it is possible to define the subspace of initial space of KPPs in which the given set of requirements to splat is fulfilled. It is the basis for computer-aided design of coatings and it allows to physically justify formulated requirements to equipment and spraying mode. For calculation of thickness of individual splats in the vicinity of the stagnation point at impact with the base of metals droplets, oxide ceramics and cermets droplets at the preset values of KPPs, the experimentally approved models [2–4] are used. Cylinder approximation for final splat morphology, as well as equality of volumes of droplet and splat, allow finding the final diameter of splat (figure 1(a)). Besides, in the course of modeling of coating formation an opportunity for carrying out the deposition of equivalent splats with smooth periphery (further named “smooth splat”) is realized in the software (figure 1(b)). For this purpose, as well as in the previous case, thickness of splats in the vicinity of stagnation point at spreading and solidification of droplet is calculated according to [2–4].

The “COATING” subsystem is based on an algorithm of stochastic laying of splats on the base with the surface geometry changing at spraying (Monte-Carlo method), therefore lamellar structure of coating is formed.

Figure 1. Microsections of model splats: **(a)** – cylindrical; **(b)** – equivalent smooth.

The use of specified two geometrical representations of splat (figure 1) allows estimating their influence on properties and structure of coatings on micro- and macrolevel (see figures 2–4 and figure 10). As it was noted above, in the absence of systematization of the experimental data and comprehensive approved idea of interrelation between the spraying modes and functional characteristics of the obtained coatings, the developed computational technology gives the chance to design them, estimate their functional characteristics (porosity structure, roughness, bonding strength with the substrate, cohesive interlayer bonding strength, etc.). Results of modeling the lamellar structure of coatings sprayed from corundum powder (α-phase of Al_2O_3) which is widely used at thermal spraying of wear-resistant, heat-protective, insulating, etc. are given below.

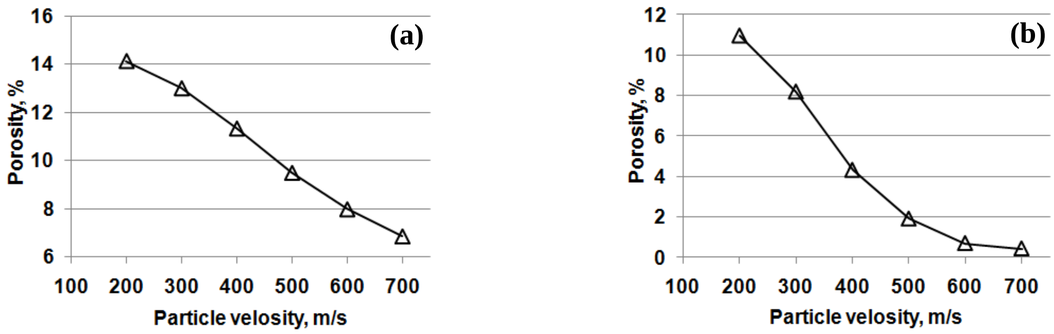

Figure 2. Porosity *P* of corundum coatings vs. velocity of particles U_p: **(a)** – cylinder approximation; **(b)** – smooth splat approximation.

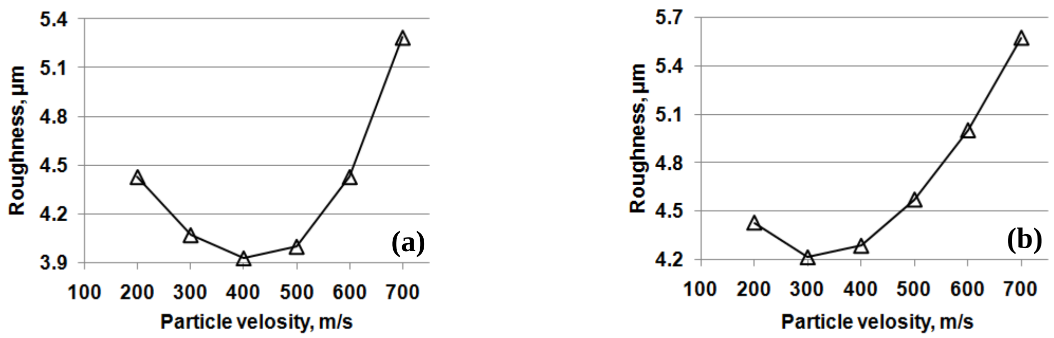

Figure 3. Roughness R_a of corundum coatings vs. velocity of particles U_p: **(a)** – cylinder approximation; **(b)** – smooth splat approximation.

Figures 2, 4 confirm the fact that when using splat geometry in the form of thin cylinder, in comparison with smooth splat approximation, coatings porosity is always overestimated in comparison with the experiment [5, 6]. Therefore, results of calculations only for smooth splat morphology are given bellow in figures 5–8. Calculations of roughness of coatings carried out, with other things being equal, for two model morphologies of splats agree both qualitatively and quantitatively (figure 3). The results of modeling presented in figures 2, 3 are obtained at the following KPPs values: temperature of particles

T_{p0} = 2330 K, diameter of particles D_p = 24 µm, temperature of steel substrate (St. 45) T_{b0} = 400 K, thickness of coatings H = 300 µm. The following KPPs values correspond to the results presented in figures 4, 5: diameter of particles D_p = 24 µm, temperature of steel substrate (St. 45) T_{b0} = 400 K, thickness of coatings H = 300 µm. For plasma spraying (APS) the velocity of particles is U_p = 200 m/s, for detonation and supersonic flame spraying (HVOF) – U_p = 627 m/s. The following KPPs values correspond to the results presented in figures 6, 7: temperature of particles T_{p0} = 2330 K, temperature of substrate (St. 45) T_{b0} = 400 K, thickness of coatings H = 300 µm. For plasma spraying the velocity of particles is U_p = 200 m/s, for a high-velocity spraying – U_p = 627 m/s.

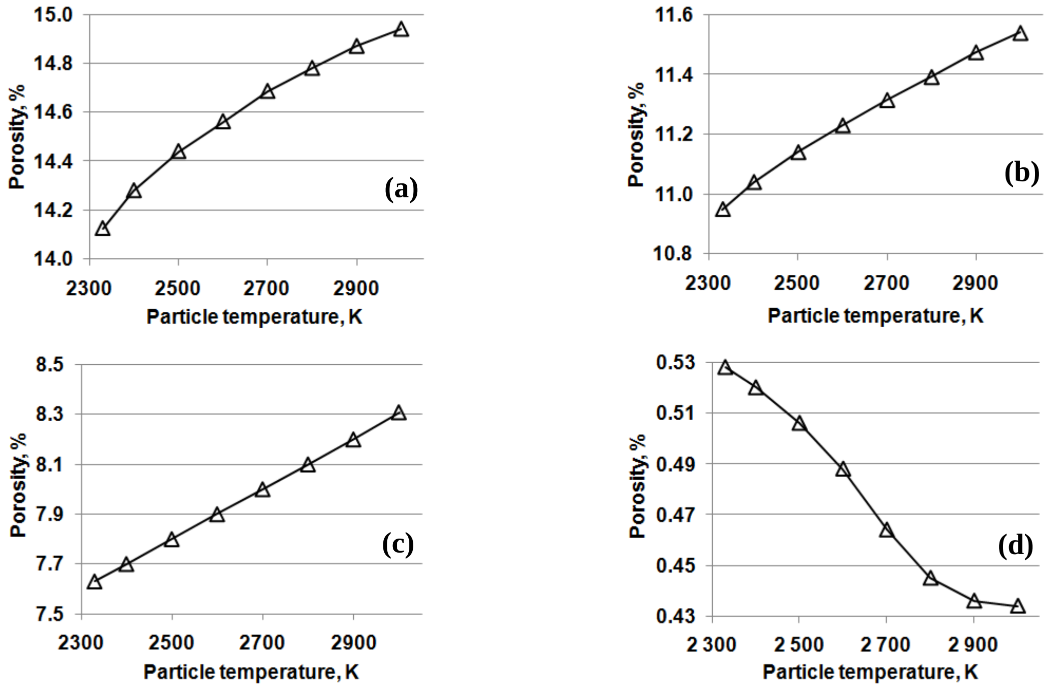

Figure 4. Porosity P of corundum coatings vs. temperature of particles T_{p0}. APS (U_p = 200 m/s): **(a)** – cylinder approximation; **(b)** – smooth splat approximation. HVOF (U_p = 627 m/s): **(c)** – cylinder approximation; **(d)** – smooth splat approximation.

The following conditions of spraying correspond to the results of modeling presented in figure 8: temperature of particles T_{p0} = 2330 K, diameter of particles D_p = 24 µm, substrate – steel (St. 45), thickness of coatings H = 300 µm. For the APS plasma mode, the velocity of particles is U_p = 200 m/s, and for the HVOF mode – U_p = 627 m/s. Under the same conditions, the roughness of coatings also changes slightly and its mean value, respectively, equals: R_a ~ 4.55 µm (APS) and R_a ~ 6.1 µm (HVOF).

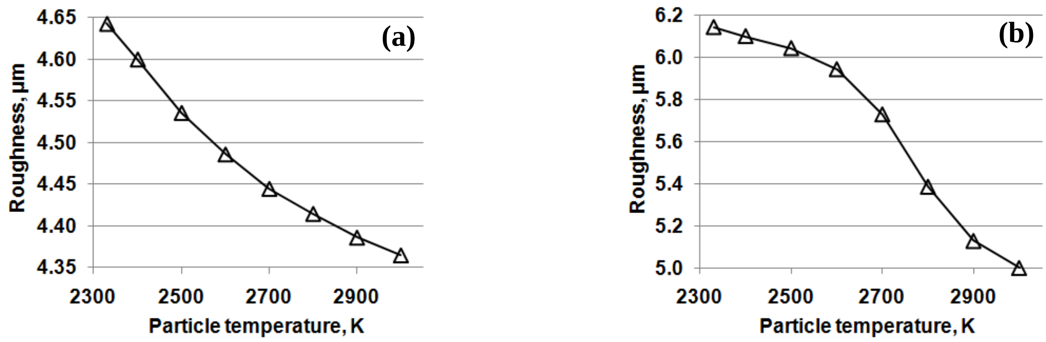

Figure 5. Roughness R_a of corundum coatings vs. temperature of particles T_{p0} (smooth splat): **(a)** – APS (U_p = 200 m/s); **(b)** – HVOF (U_p = 627 m/s).

The microsections of two plasma coatings illustrating, all other things being equal, distinctions in porosity structure when using two model morphologies of splats (figure 1) are given in figure 9. The porosity of coating (figure 9(a)) obtained with the use of cylinder approximation equals 14.7 % according to figure 4(a) and is overestimated in comparison with the experimental value of 11 % given in [5]. In turn, the porosity of coating (figure 9(b)) obtained with the use of smooth splat approximation equals 11.3 % (figure 4(b)), which agrees with the experiment [5].

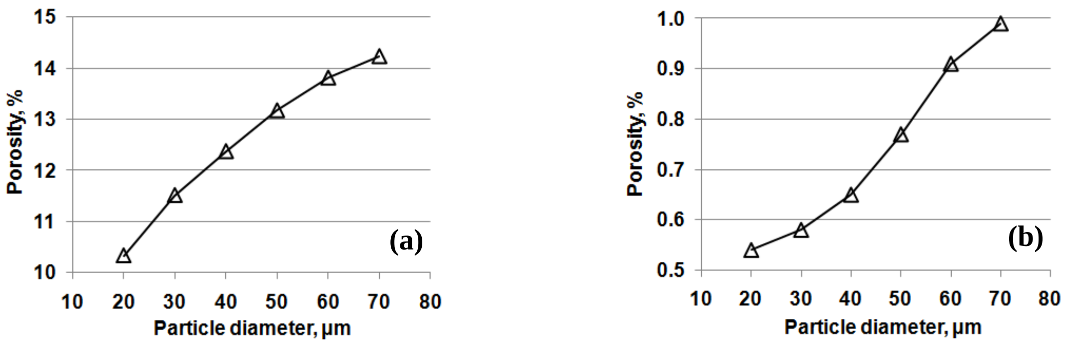

Figure 6. Porosity P of corundum coatings vs. diameter of particles D_p (smooth splat): **(a)** – APS ($U_p = 200$ m/s); **(b)** – HVOF ($U_p = 627$ m/s).

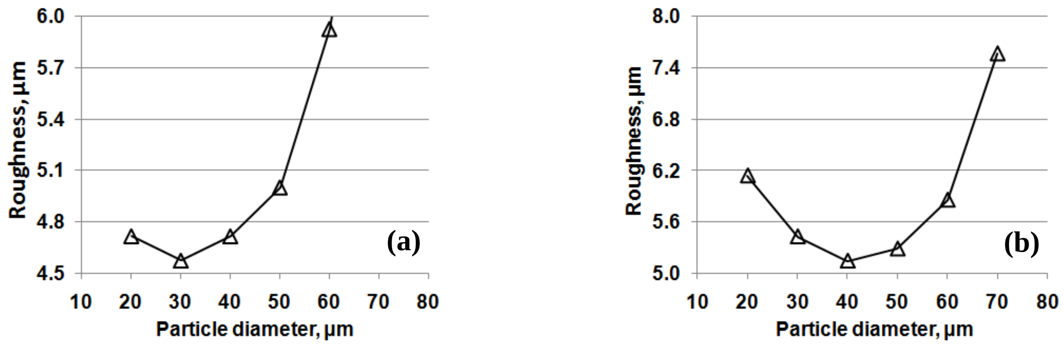

Figure 7. Roughness R_a of corundum coatings vs. diameter of particles D_p (smooth splat): **(a)** – APS ($U_p = 200$ m/s); **(b)** – HVOF ($U_p = 627$ m/s).

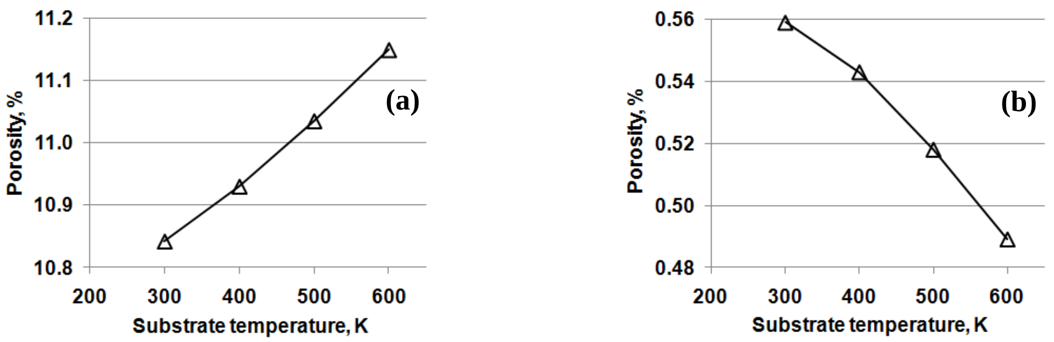

Figure 8. Porosity P of corundum coatings vs. substrate temperature T_{b0} (smooth splat): **(a)** – APS ($U_p = 200$ m/s); **(b)** – HVOF ($U_p = 627$ m/s).

The confirmation of validity of coatings modeling with use of the second model morphology of splat for detonation spraying conditions ($T_{p0} = 2330$ K, $U_p = 627$ m/s, $D_p = 24$ µm, $T_{b0} = 400$ K, thickness of coatings $H = 300$ µm) is the calculated value of porosity $P = 0.53$ % which almost agrees with the experimental value $P = 0.6$ % of the paper [6].

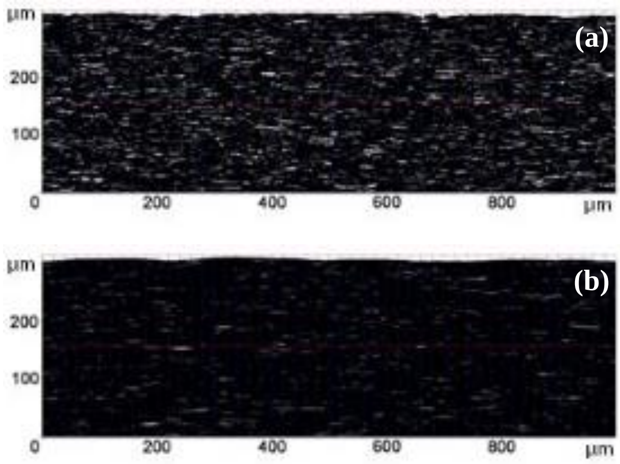

Figure 9. Microsections of plasma coatings from the corundum powder at KPPs values: U_p = 200 m/s, T_{p0} = 2700 K, D_p = 24 µm, temperature of steel substrate (St. 45) T_{b0} = 400 K: **(a)** – cylinder approximation; **(b)** – smooth splat approximation.

References

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