Prediction of the functional characteristics of plasma titanium aluminide coatings by computer simulation

V I Jordan\textsuperscript{1,2} and V A Blednov\textsuperscript{2}

\textsuperscript{1}Department of Computing Techniques and Electronics, Altai State University, 61, Lenina ave., Barnaul, 656049, Russia
\textsuperscript{2}Khristianovich Institute of Theoretical and Applied Mechanics, Siberian Branch of RAS, 4/1, Institutskaya str., Novosibirsk, 630090, Russia

E-mail: jordan@phys.asu.ru, ihammers.sia@gmail.com

Abstract. The results of stochastic simulation (computer-aided design) of a layered structure formation and functional characteristics (porosity, roughness, adhesion) of metal coatings based on titanium aluminide powders ($\gamma$-phase TiAl) under conditions typical of atmospheric plasma spraying are given. Taking into account the stable formation of a metal splats and titanium aluminide coatings, as well as minimum porosity and maximum adhesive strength of coatings, the optimal plasma spraying mode has been obtained: the particle velocity $U_p = 250$ m/s, the particle temperature $T_p \leq 2050$ K, the particle diameter $D_p = (30 \pm 10)$ $\mu$m.

1. Introduction

Intermetallic alloys like titanium aluminides, for example, TiAl$_3$, TiAl, Ti$_3$Al, can be pretended to as promising structural materials. The combination of low density, strength properties, high corrosion resistance, heat resistance and high-temperature strength makes them very attractive for various areas of engineering, including in aeronautical engineering and aerospace engineering to create protective coatings as widespread structural materials [1]. TiAl-based alloys are promising materials for the manufacture of pipes, supports, compressor housings, low-pressure air chambers filters, nozzles, compressor blades and turbines of aircraft engines, as well as for the manufacture of shell elements of spacecraft and elements of thermal protection systems of hypersonic aircraft. The intermetallic compound TiAl is used to manufacture exhaust valves, turbocharger parts and other automotive engine components, instead of heat resistant stainless steels and nickel alloys.

However, titanium aluminides, like most intermetallic compounds, are characterized by “embrittlement” in a wide range of temperatures, which reduces the range of their practical application in mechanical engineering as structural materials. The increase in the mechanical properties of the TiAl compound is achieved by doping this alloy with the following elements: Hf, Mo, Nb, Ta, V, W, Zr. For example, the deposition on turbine blades of aircraft engines of wear-resistant coatings of Ti-43.5%Al-4.5%Nb-1.7%Mo alloy (component concentration in at.\%) ensures reliability and durability at temperatures from 650 to 900 °C [2].

When spraying such coatings with gas-thermal methods (plasma, detonation, HVOF, etc.), an important aspect is the study of ways to control the phase composition and microstructure of coatings for such systems chemically sensitive to the detonation products of a fuel-oxygen gas mixture, as well as for composite materials in which chemical interaction between phases is possible at elevated temperatures that are characteristic for the detonation spraying. In the spraying process of titanium
aluminides coatings the oxidation reactions are undesirable [3]. The formation of new intermetallic phases increases the hardness of coatings. The TiAl compound partially decomposes to form Ti3Al, which under the conditions of spraying undergoes a slight decomposition, but is not exposed to nitrogen. For spraying of coatings based on TiAl, Ti3Al and TiAl3 intermetallic compounds, powders with fractions in the range of 0–70 μm are used. Coatings, in the formation of which chemical reactions are involved, acquire a hierarchical structure with practically unchanged chemical composition of the phases in the coatings, but the relative content of the phases may be change [3].

2. Procedure of the computational experiments
For simulation (computer-aided design) the layered structure of coatings and predicting their functional characteristics, a previously developed and user-proven software package was used (a software system for parallel execution of a cycle of computational experiments with different sets of “key physical parameters (KPPs)” of sprayed particles of powder and substrate). The simulation procedure implements the approach of stochastic particle spraying (Monte-Carlo method) taking into account the changing relief of the sprayed surface based on experimentally tested theoretical solutions that adequately implement conjugate processes and features of the hydrodynamic spreading of a particle melt at the point of impact with the surface and the processes of solidification of the particle melts spreading on the sprayed surface (so-called “splats”, [4–7]). In this case, four scenarios for the formation of splat are possible: 1. spreading and simultaneous solidification of the droplet on the solid base; 2. spreading and simultaneous solidification of the droplet, and local submelting of the base at the contact spot with the droplet; 3. spreading of the droplet over the solid base surface, and subsequent cooling and solidification of the spread layer; 4. spreading of the droplet accompanied with simultaneous local submelting of the base, followed by subsequent cooling and solidification of both.

In computational experiments of the coatings simulation based on the γ-phase of TiAl, a 2x2 mm plate made of 45 grade steel was used as a substrate (the substrate temperature is 400 K). In practical terms, the thermophysical properties of TiAl (as well as density, dynamic viscosity, etc) slightly differ from similar properties of the doped alloy Ti-43.5%Al-4.5%Nb-1.7%Mo, therefore the simulation results (they show below in the table 1 for two compositions) can be considered general within the error of the characteristics prediction (about 3-5%). With a change in the particle temperature Tp in the range from 1750 to 2150 K, the average value of the particle diameter Dp was kept equal to 30 μm in 2-speed plasma spraying modes (Up = 200 and 250 m/s). In addition, in these 2-speed plasma spraying modes at a constant temperature of 1750 K (slightly above the melting temperature of the γ-phase TiAl from 1720 - 1730 K), the particle diameter Dp changed from 20 to 70 μm.

3. Results of the computational experiments
The results of the coatings simulation (100 μm of thick) are summarized in a single table 1, in which, in addition to the characteristics of the coatings, the "key physical parameters (KPPs)" of the powder particles corresponding to them is given. In the table 1, besides designating the splat diameter Ds, expressed in microns, there is a normalized value of the splat diameter \( \bar{D}_s = D_s / D_p \), expressed in relative units (r.u.) and which is otherwise called "the spreading factor" of melt particle. For metal splats, the value of the spreading factor should not exceed the value of 4.5 (starting from value 5, the integrity of the splat shape is not guaranteed, [8]). Along with the splat thickness \( \bar{h}_s = h_s / D_p \), the normalized value of the splat thickness \( \bar{h}_s = h_s / D_p \) is given. Value \( P\% \) denotes the coating porosity, and value \( R_u \) denotes the surface roughness parameter of the coating. The \( \sigma_{\text{adg}} \) value is the relative adhesion strength – the bonding strength of the first coating monolayer to the substrate (in other words, the ratio of the absolute adhesion strength of the TiAl coating to the tensile strength for the intermetallic compound TiAl, i.e. it is the fraction of maximum possible value of the absolute adhesion strength, with equal 1100 MPa [3]). The \( T_c \) value shows the temperature of contact at the point of collision of the melt particle with the surface.
Table 1. Particle parameters and coating characteristics.

| $T_p$, K | $U_p$, m/s | $D_{p0}$, μm | $D_s$, μm | $h_{s0}$, μm | $H_{s0}$, r.u. | $P$, % | $R_{x}$, μm | $\sigma_{alg}$, r.u. | $T_c$, K | Scen. |
|---------|-----------|-------------|---------|-------------|--------------|------|-----------|---------------|--------|------|
| 1750    | 200       | 30          | 101     | 3.366       | 1.77         | 0.059| 10.02     | 1.74          | 0.0002 | 1160 | 1     |
| 1850    | 200       | 30          | 106     | 3.525       | 1.61         | 0.054| 9.95      | 1.65          | 0.0004 | 1195 | 1     |
| 1950    | 200       | 30          | 111     | 3.701       | 1.46         | 0.049| 8.04      | 1.63          | 0.0006 | 1236 | 1→3   |
| 2050    | 200       | 30          | 117     | 3.899       | 1.32         | 0.044| 7.91      | 1.60          | 0.0014 | 1278 | 1→3   |
| 2150    | 200       | 30          | 181     | 6.028       | 0.55         | 0.018| 8.02      | 1.55          | 0.1000 | 1339 | 3     |
| 1750    | 200       | 20          | 61      | 3.052       | 1.43         | 0.072| 8.92      | 1.54          | 0.0001 | 1160 | 1     |
| 1750    | 200       | 40          | 144     | 3.609       | 2.05         | 0.051| 10.25     | 2.06          | 0.0003 | 1160 | 1     |
| 1750    | 200       | 50          | 191     | 3.811       | 2.29         | 0.046| 10.32     | 2.98          | 0.0003 | 1339 | 1→3   |
| 1750    | 200       | 60          | 239     | 3.985       | 2.52         | 0.042| 10.49     | 3.91          | 0.0003 | 1339 | 1→3   |
| 1750    | 200       | 70          | 500     | 7.141       | 0.92         | 0.013| 10.91     | 6.09          | 0.0106 | 1339 | 3     |
| 1750    | 250       | 30          | 107     | 3.553       | 1.58         | 0.053| 8.26      | 1.68          | 0.0002 | 1160 | 1     |
| 1850    | 250       | 30          | 112     | 3.721       | 1.44         | 0.048| 8.12      | 1.45          | 0.0004 | 1200 | 1     |
| 1950    | 250       | 30          | 117     | 3.909       | 1.31         | 0.044| 4.73      | 1.91          | 0.0005 | 1478 | 1→3   |
| 2050    | 250       | 30          | 189     | 6.303       | 0.50         | 0.017| 4.67      | 1.85          | 0.0397 | 1548 | 3     |
| 2150    | 250       | 30          | 189     | 6.303       | 0.50         | 0.017| 4.82      | 1.94          | 0.0749 | 1618 | 3     |
| 1750    | 250       | 20          | 64      | 3.220       | 1.29         | 0.064| 8.15      | 1.39          | 0.0001 | 1160 | 1     |
| 1750    | 250       | 40          | 152     | 3.811       | 1.84         | 0.046| 5.60      | 2.41          | 0.0002 | 1339 | 1→3   |
| 1750    | 250       | 50          | 201     | 4.025       | 2.06         | 0.041| 6.15      | 3.17          | 0.0002 | 1339 | 1→3   |
| 1750    | 250       | 60          | 434     | 7.240       | 0.76         | 0.013| 6.95      | 4.56          | 0.0074 | 1339 | 3     |
| 1750    | 250       | 70          | 523     | 7.467       | 0.84         | 0.012| 8.49      | 5.83          | 0.0087 | 1339 | 3     |

As shown in the table 1, at the transition from the first layer to the next, the scenario of melt particle spreading can be changed, for example, 1→3. Based on the data in the table 1, graphical dependencies of coating porosity vs. temperature and particle diameter are plotted for two values of particle velocity (figures 1, 2), as well as temperature dependencies of adhesive strength of the coating to the substrate (figure 3) for the same two values of particle velocity.

Analyzing the last column “Scenario” in the table 1, it is clear that the transition from the first to the third scenario of the melt particle spreading is accompanied by a noticeable increase in the contact
An increase in the adhesive strength of the coatings is a direct consequence of an increase in the contact temperature $T_c$. From the table 1 (as well as from figures 1 and 3) it can be seen that the increase in $T_c$ (transition 1→3) for both spraying modes ($U_p = 200$ and 250 m/s) occurs when the temperature of particles $T_p$ exceeds 1950 K. Therefore, at temperatures of particles $T_p$ over 1950 K there is a significant increase in the adhesive strength of the coatings (figure 3). In addition, at temperatures of particles $T_p$ above 1950 K, the tendency of a sharp decrease in the porosity of the coatings (figure 1) changes to a tendency of practically no noticeable increase.

**Figure 1.** Temperature dependencies of coating porosity $P\%$ for two values of particle velocity: (a) – the particle velocity $U_p = 200$ m/s; (b) – the particle velocity $U_p = 250$ m/s.

**Figure 2.** Dependences of coating porosity $P\%$ vs. particle diameter $D_p$ for two values of particle velocity: (a) – the particle velocity $U_p = 200$ m/s; (b) – the particle velocity $U_p = 250$ m/s.

**Figure 3.** Temperature dependencies of adhesive strength of the coating to the substrate for two values of particle velocity: (a) – the particle velocity $U_p = 200$ m/s; (b) – the particle velocity $U_p = 250$ m/s.

Also from the table 1 and from figure 2 it can be seen that the increase in $T_c$ (transition 1→3) for both spraying modes ($U_p = 200$ and 250 m/s) occurs when the particle diameter $D_p$ exceeds 40 μm. The
tendency to an increase in the porosity of the coatings is almost the same for both modes ($U_p = 200$ and $250 \text{ m/s}$), but different for particle diameter values in the range of $20–40 \mu\text{m}$. For the first spraying mode ($U_p = 200 \text{ m/s}$) and for particle diameter values in the range of $20–40 \mu\text{m}$, the coatings porosity also increases as for particle diameter values above $40 \mu\text{m}$. However in the second mode ($U_p = 250 \text{ m/s}$) the coating porosity values drops for particle diameter values in the range of $30–40 \mu\text{m}$. The second spraying mode ($U_p = 250 \text{ m/s}$) is preferable to the first one, since, as a whole, the coating porosity values in the second mode are significantly lower than in the first one.

4. Conclusion

The software package developed by the authors is implemented as a software system with parallel launching of SIMD tasks for simulation gas-thermal coatings with different KPPs sets of particles. The possibility of parallel computing allows you to perform a large cycle of computational experiments and establish the relationship between spraying modes and functional operational characteristics of coatings.

Taking into account the stable formation of a metal splats ($\overline{D} \leq 5\%$) and titanium aluminide coatings, as well as minimum porosity and maximum adhesive strength of coatings, the optimal plasma spraying mode has been obtained: the particle velocity $U_p = 250 \text{ m/s}$, the particle temperature $T_p \leq 2050 \text{ K}$, the particle diameter $D_p = (30 \pm 10) \mu\text{m}$.

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