Computer-aided detection of the optimal spraying modes of coatings based on intermetallic titanium-aluminum alloys

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Abstract. The computational experiments results on simulation of a layered structure formation and the prediction of characteristics (porosity, roughness, adhesion) of metallic coatings based on intermetallic titanium-aluminum alloys (α₂-Ti₃Al, γ-TiAl and TiAl₃) are given. The coatings under conditions typical of atmospheric plasma spraying (APS) and for high-velocity spraying (HVOF, D-Gun Spraying, etc.) by computer-aided design have been prepared. The ranges of the “key physical parameters (KPPs)” values of the sprayed particles, which ensure the stable formation of spreading and solidified melt particles (splats) on the sprayed surface for each of the three types of intermetallic titanium-aluminum coatings, have been detected. Taking into account the stable splat formation conditions, as well as the minimum of porosity (and roughness) and the maximum adhesion strength of the simulated coatings, the optimal spraying modes of coatings based on intermetallic titanium-aluminum alloys (Ti₃Al, TiAl and TiAl₃) were determined.

1. Introduction

Currently, alloys based on the intermetallic compounds of Ti₃Al, TiAl and TiAl₃ are considered as promising structural materials due to their low density, strength properties, high corrosion resistance, heat resistance and high-temperature strength. These properties make them very attractive for various areas of engineering, including in aeronautical engineering and aerospace engineering to create protective coatings as widespread structural materials [1]. Ti₃Al-based and TiAl-based alloys are used for the manufacture of structural elements of aircraft engines, as well as for the manufacture of shell elements of spacecraft and elements of thermal protection systems hypersonic aircraft. In addition, the intermetallic TiAl-compound is used to manufacture structural elements of automotive engines and instead of heat-resistant stainless steels and nickel alloys.

Like most intermetallic compounds, titanium-aluminum 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 improvement of the mechanical properties of titanium-aluminum intermetallic compounds is achieved by doping these alloys with the following elements: Hf, Mo, Nb, Ta, V, W, Cr, Zr. Wear-resistant coatings of Ti–43.5%Al–4.5%Nb–...
1.7%Mo alloy (concentration in at.%) are applied to the turbine blades of aircraft engines, as a result of which reliability and durability are achieved at temperatures from 650 to 900 °C [2].

In addition, Ti–48%Al–2%Cr–2%Nb alloy is one of the best alloys based on TiAl. This alloy has a good combination of plasticity and adaptability, high efficiency of heat resistance, corrosion resistance [3]. The Ti–22%Al–1.5%Nb–0.25%Cu alloy (concentration in wt.%) based on the Ti₃Al-intermetallic belongs to domestic alloys and has a positive effect on the strength and ductility of the alloy [3].

When spraying with gas-thermal methods (APS, D-Gun Spraying, HVOF, etc.) of coatings based on titanium-aluminum intermetallic alloys, it is necessary to solve the problem of controlling the phase composition and microstructure of coatings for such systems chemically sensitive to detonation products of the fuel-oxygen gas mixture, and take into account the possible chemical interaction between the phases at elevated temperatures characteristic of detonation spraying. When spraying intermetallic coatings based on TiAl, Ti₃Al and TiAl₁₃, powders with fractions in the range of 0-70 microns are used. Taking into account chemical reactions, the hierarchical structure of intermetallic phases is formed with practically unchanged chemical composition of the phases in the coatings, but the relative content of the phases may be vary [4].

2. Methodical features of coatings simulation and parametric conditions for computational experiments (CEs)

For simulation (computer-aided design) the layered structure of coatings and predicting their functional characteristics, a software package developed and tested by the authors, more precisely, a software system for parallel execution of a cycle of CEs with various sets of initial “key physical parameters (KPPs)” of sprayed particles and substrate was used. The simulation technique is based on the stochastic approach of particle spraying (Monte-Carlo method), taking into account the changing topography of the sprayed surface and the generators of “pseudo-random” numbers that implement the statistical distribution laws of the KPPs for particles. In addition, based on experimentally tested theoretical solutions, the features of the hydrodynamic spreading of a particle melt at the points of impact with the surface and the processes of solidification of the particle melts spreading on the sprayed surface (so-called “splat”, [5-8]). These features characterize four possible scenarios for the formation of splats: 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 CEs for the computer-aided design of three types of coatings (based on the Ti₃Al, TiAl and TiAl₁₃ compounds), a 2x2 mm plate made of 45 grade steel was used as the substrate (the substrate temperature is 400 K). In practical terms, the thermophysical properties of Ti₃Al (as well as density, dynamic viscosity, etc.) differ slightly from the analogous properties of the Ti–22%Al–1.5%Nb–0.25%Cu doped alloy (concentration in wt.%). Therefore the simulation results of the Ti₃Al-coatings and coatings based on an alloy close in composition to Ti₃Al can be considered common within the error of the simulation characteristics (about 3-5%). The situation is similar for Ti–43.5%Al–4.5%Nb–1.7%Mo and Ti–48%Al–2%Cr–2%Nb alloys (concentration in at.%), which by their thermophysical properties (as well as density and viscosity, etc.) comparable to TiAl intermetal compound. Of interest is also the prediction of the coatings properties based on the TiAl₁₃ intermetallic compound in comparison with the coatings properties based on the Ti₃Al and TiAl intermetallic compounds.

In CEs, when simulated the coatings based on Ti₃Al, the particle temperature $T_p$ varied in the range from 1450 to 1850 K (the melting temperature of the $α_2$-phase Ti₃Al is about 1430 K); to simulate the coatings based on TiAl, the particle temperature $T_p$ changed from 1750 to 2150 K (the melting point of the $γ$-phase TiAl is about 1733 K) and for coatings simulation based on TiAl₁₃, the particle temperature $T_p$ varied in the range from 1700 to 2100 K (the melting temperature of the TiAl₁₃ compound is about 1668 K). The average particle diameter $D_p$ was maintained at 30 µm in plasma spraying modes ($U_p = 200$ and 250 m/s) and high-velocity modes ($U_p = 500$, 600 and 700 m/s). In addition, experiments were
carried out at varying the particle diameter $D_p$ in the range from 20 to 70 $\mu$m. At the same time, the particle temperature values were fixed: 1450 K – for Ti$_3$Al, 1750 K – for TiAl, 1700 K – for TiAl$_3$.

3. Analysis of computational experiments results

The results of the coatings simulation (100 $\mu$m thick) based on the Ti$_3$Al, TiAl and TiAl$_3$ intermetallic compounds are summarized in tables 1, 2, 3 and 4, in which, besides the coatings characteristics, the corresponding KPPs of powder particles are given. In the tables below (tables 1, 2, 3 and 4) there are designations of the splat diameter $D_s$, expressed in microns, and the normalized value of the splat diameter $\overline{D}_s = D_s / D_p$, expressed in relative units (r.u.). The $\overline{D}_s$ value is otherwise called "the spreading factor" of melt particle. The spreading factor value for metal splats should not exceed the value of 4.5 (starting from 5, the integrity of the splat shape is not guaranteed, [9]). Along with the splat thickness $h_s$, the tables give the normalized thickness $\overline{h}_s = h_s / D_p$, value $P\%$ indicates the coating porosity, and $R_s$ denotes the surface roughness parameter of the coating. The $\overline{\sigma}_{adg}$ 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 adhesive strength of the coating to the tensile strength for the intermetallic compound which is the base of coating), i.e. $\overline{\sigma}_{adg}$ - the fraction of the maximum possible adhesive strength.

**Table 1.** Particle parameters and characteristics of Ti$_3$Al-coatings sprayed by the APS method.

| $T_p$, K | $U_p$, m/s | $D_0$, $\mu$m | $D_s$, $\mu$m | $\overline{D}_s$, r.u. | $h_s$, $\mu$m | $\overline{h}_s$, r.u. | $P\%$ | $R_s$, $\mu$m | $\overline{\sigma}_{adg}$, r.u. | $T_{cv}$, K | Scenario |
|---------|------------|----------------|---------------|-----------------|-------------|--------|-------|-------------|----------------|-----------|---------|
| 1450    | 100        | 30             | 107           | 3.556           | 1.58        | 0.053  | 12.53 | 1.767       | 0.00003        | 1022      | 1       |
| 1550    | 100        | 30             | 113           | 3.782           | 1.40        | 0.047  | 13.78 | 1.538       | 0.00006        | 1200      | 1→3     |
| 1650    | 100        | 30             | 121           | 4.043           | 1.22        | 0.041  | 13.92 | 1.430       | 0.00002        | 1270      | 1→3     |
| 1750    | 100        | 30             | 156           | 5.186           | 0.74        | 0.025  | 13.85 | 1.575       | 0.0089         | 1339      | 3       |
| 1850    | 100        | 30             | 156           | 5.186           | 0.74        | 0.025  | 13.82 | 1.554       | 0.0203         | 1409      | 3       |
| 1450    | 100        | 20             | 64            | 3.223           | 1.28        | 0.064  | 11.14 | 1.480       | 0.00002        | 1022      | 1       |
| 1450    | 100        | 40             | 153           | 3.815           | 1.83        | 0.046  | 15.10 | 2.208       | 0.00003        | 1130      | 1→3     |
| 1450    | 100        | 50             | 201           | 4.028           | 2.05        | 0.041  | 15.79 | 3.048       | 0.00004        | 1130      | 1→3     |
| 1450    | 100        | 60             | 357           | 5.957           | 1.13        | 0.019  | 15.40 | 3.665       | 0.00007        | 1130      | 3       |
| 1450    | 100        | 70             | 430           | 6.144           | 1.24        | 0.018  | 15.61 | 5.253       | 0.00009        | 1130      | 3       |
| 1450    | 150        | 30             | 118           | 3.926           | 1.30        | 0.043  | 11.33 | 1.581       | 0.00002        | 1130      | 1→3     |
| 1550    | 150        | 30             | 169           | 5.624           | 0.63        | 0.021  | 11.02 | 1.537       | 0.00077        | 1200      | 3       |
| 1650    | 150        | 30             | 169           | 5.624           | 0.63        | 0.021  | 11.18 | 1.444       | 0.00235        | 1270      | 3       |
| 1750    | 150        | 30             | 169           | 5.624           | 0.63        | 0.021  | 11.25 | 1.508       | 0.00574        | 1339      | 3       |
| 1850    | 150        | 30             | 169           | 5.624           | 0.63        | 0.021  | 11.14 | 1.565       | 0.01357        | 1409      | 3       |
| 1450    | 150        | 20             | 71            | 3.556           | 1.05        | 0.053  | 10.84 | 1.485       | 0.00001        | 1022      | 1       |
| 1450    | 150        | 40             | 238           | 5.957           | 0.75        | 0.019  | 12.04 | 2.370       | 0.00033        | 1131      | 3       |
| 1450    | 150        | 50             | 311           | 6.229           | 0.86        | 0.017  | 12.82 | 3.229       | 0.00045        | 1131      | 3       |
| 1450    | 150        | 60             | 388           | 6.461           | 0.96        | 0.016  | 13.24 | 4.168       | 0.00051        | 1131      | 3       |
| 1450    | 150        | 70             | 466           | 6.663           | 1.05        | 0.015  | 14.22 | 5.675       | 0.00059        | 1131      | 3       |
| 1450    | 500        | 30             | 215           | 7.156           | 0.39        | 0.013  | 0.93  | 0.552       | 0.00007        | 962       | 3       |

The tensile strength of TiAl compound is 1100 MPa [4] and the tensile strength of Ti$_3$Al compound is
of the same order (ca to 1000 MPa [3]). A comparison of the Ti₃Al, TiAl and TiAl₃ phases by microhardness [1] allows us to obtain for the TiAl₃ phase an indirect estimate of the tensile strength of about 500 MPa. The $T_c$ value in the tables shows the contact temperature at the collision point of the melt particle with the surface (in the first layer of the coating – with the substrate, and in the next layers – with the sprayed layer of the same particles).

Table 2. Particle parameters and characteristics of TiAl-coatings sprayed by the APS method.

| $T_p$, K | $U_p$, m/s | $D_p$, μm | $D_s$, μm | $\bar{D}_s$, r.u. | $h_s$, μm | $\bar{h}_s$, r.u. | $P_r$, % | $R_{sl}$, μm | $\bar{\tau}_{adg}$, r.u. | $T_c$, K | Scenario |
|---------|------------|-----------|-----------|-----------------|----------|---------------|-----|-------------|--------------|---------|---------|
| 1750    | 200        | 30        | 101       | 3.366           | 1.77     | 0.059         | 10.02 | 1.740       | 0.0002       | 1160    | 1       |
| 1850    | 200        | 30        | 106       | 3.525           | 1.61     | 0.054         | 9.95  | 1.648       | 0.0004       | 1195    | 1       |
| 1950    | 200        | 30        | 111       | 3.701           | 1.46     | 0.049         | 8.04  | 1.633       | 0.0006       | 1236    | 1→3     |
| 2050    | 200        | 30        | 117       | 3.899           | 1.32     | 0.044         | 7.91  | 1.600       | 0.0014       | 1278    | 1→3     |
| 2150    | 200        | 30        | 181       | 6.028           | 0.55     | 0.018         | 8.02  | 1.551       | 0.1000       | 1339    | 3       |
| 1750    | 200        | 60        | 239       | 3.985           | 2.52     | 0.042         | 10.49 | 3.908       | 0.0003       | 1339    | 1→3     |
| 1750    | 200        | 70        | 500       | 7.141           | 0.92     | 0.013         | 10.91 | 6.091       | 0.0106       | 1339    | 3       |
| 1750    | 250        | 30        | 107       | 3.553           | 1.58     | 0.053         | 8.26  | 1.682       | 0.0002       | 1160    | 1       |
| 1850    | 250        | 30        | 112       | 3.721           | 1.44     | 0.048         | 8.12  | 1.445       | 0.0004       | 1200    | 1       |
| 1950    | 250        | 30        | 117       | 3.909           | 1.31     | 0.044         | 4.73  | 1.905       | 0.0005       | 1478    | 1→3     |
| 2050    | 250        | 30        | 189       | 6.303           | 0.50     | 0.017         | 4.67  | 1.845       | 0.0397       | 1548    | 3       |
| 2150    | 250        | 30        | 189       | 6.303           | 0.50     | 0.017         | 4.82  | 1.940       | 0.0749       | 1618    | 3       |
| 1750    | 250        | 20        | 64        | 3.220           | 1.29     | 0.064         | 8.15  | 1.394       | 0.0001       | 1160    | 1       |
| 1750    | 250        | 40        | 152       | 3.811           | 1.84     | 0.046         | 5.60  | 2.412       | 0.0002       | 1339    | 1→3     |
| 1750    | 250        | 50        | 201       | 4.025           | 2.06     | 0.041         | 6.15  | 3.167       | 0.0002       | 1339    | 1→3     |
| 1750    | 250        | 60        | 434       | 7.240           | 0.76     | 0.013         | 6.95  | 4.560       | 0.0074       | 1339    | 3       |
| 1750    | 250        | 70        | 523       | 7.467           | 0.84     | 0.012         | 8.49  | 5.826       | 0.0087       | 1339    | 3       |
| 1750    | 500        | 30        | 217       | 7.240           | 0.38     | 0.013         | 0.85  | 0.470       | 0.002        | 1160    | 1→3     |

Table 3. Particle parameters and characteristics of TiAl₃-coatings sprayed by the APS method.

| $T_p$, K | $U_p$, m/s | $D_p$, μm | $D_s$, μm | $\bar{D}_s$, r.u. | $h_s$, μm | $\bar{h}_s$, r.u. | $P_r$, % | $R_{sl}$, μm | $\bar{\tau}_{adg}$, r.u. | $T_c$, K | Scenario |
|----------|------------|-----------|-----------|-----------------|----------|---------------|-----|-------------|--------------|---------|---------|
| 1700     | 200        | 30        | 83        | 2.781           | 2.59     | 0.086         | 8.73  | 2.374       | 0.0031       | 1105    | 1       |
| 1800     | 200        | 30        | 89        | 2.972           | 2.26     | 0.075         | 9.16  | 2.240       | 0.0062       | 1148    | 1       |
| 1900     | 200        | 30        | 96        | 3.201           | 1.95     | 0.065         | 9.51  | 1.937       | 0.0147       | 1195    | 1       |
| 2000     | 200        | 30        | 104       | 3.481           | 1.65     | 0.055         | 9.94  | 1.809       | 0.0310       | 1245    | 1       |
| 2100     | 200        | 30        | 115       | 3.834           | 1.36     | 0.045         | 10.31 | 1.525       | 0.0615       | 1299    | 1       |
| 1700     | 200        | 20        | 51        | 2.526           | 2.09     | 0.104         | 7.68  | 2.066       | 0.0019       | 1105    | 1       |
| 1700     | 200        | 40        | 119       | 2.980           | 3.00     | 0.075         | 9.29  | 2.500       | 0.0042       | 1105    | 1       |
| 1700     | 200        | 50        | 157       | 3.144           | 3.37     | 0.067         | 9.74  | 2.673       | 0.0054       | 1105    | 1       |
| 1700     | 200        | 60        | 197       | 3.286           | 3.71     | 0.062         | 9.99  | 3.020       | 0.0061       | 1105    | 1       |
As can be seen from the tables (tables 1, 2, 3 and 4), in all cases, with an increasing in the particle velocity, the coatings porosity decreases, and with an increase in the particle temperature, the adhesion strength of the coatings increases. In addition, the transition from the 1st spreading scenario of a melt...
particle to the 3rd is a direct consequence of a noticeable increase in the contact temperature $T_c$. The spreading factor values $D_s$, indicated in the last rows of tables 1 and 2 for particle velocities $U_p = 500$ m/s, significantly exceed the critical value 5. Therefore, in high-velocity spraying modes (HVOF, D-Gun Spraying, etc.) it is impossible to guarantee the stable splat formation and coatings formed on the basis of Ti$_3$Al and TiAl intermetallic compounds, as well as the coatings based on alloys close in composition to the Ti$_3$Al and TiAl intermetallic compounds. Analyzing the spreading factor values $D_s$ in tables 3 and 4, for coatings based on TiAl$_3$ compound we can conclude that for these coatings can been implemented both plasma APS spraying method and high-velocity HVOF and D-Gun spraying methods.

4. Conclusions
For the stable formation of metal splats and coatings, taking into account the conditions ($D_s < 5$), as well as conditions of minimum porosity and maximum adhesive strength of coatings, it can be considered that the following modes are optimal for spraying of coatings based on titanium-aluminum intermetallic alloys.

1. For the spraying of coatings based on Ti$_3$Al intermetallic compounds, the APS method can be implemented and its optimal mode is determined by the following particle parameters (table 1): particle velocity $U_p = 150$ m/s, particle temperature $T_p \leq 1500$ K, particle diameter $D_p = (30 \pm 10)$ μm.

2. For the spraying of coatings based on TiAl intermetallic compounds, the APS method can be implemented and its optimal mode is determined by the following particle parameters (table 2): particle velocity $U_p = 250$ m/s, particle temperature $T_p \leq 2000$ K, particle diameter $D_p = (30 \pm 10)$ μm.

3. For the spraying of coatings based on TiAl$_3$ intermetallic compounds, both the APS method and the high-velocity methods HVOF and D-Gun Spraying can be implemented. The optimal mode is determined by the following particle parameters (table 4): particle velocity $U_p = 700$ m/s, particle temperature $T_p = 1800$ K, particle diameter $D_p = (30 \pm 10)$ μm.

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.

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