Development of mathematical model of disperse particle motion in the plasma flow in the field of boundary layer during plasma spraying

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Abstract. The task of mathematical modelling of disperse particle motion in a two-phase plasma flow in the field of boundary layer for plasma coatings deposition has been solved. The model takes into account that disperse particles move along different trajectories and with different speeds. Speed change of mass center of particles in the field of boundary layer has also been considered. Components of particle mass center speed when they fall on the surface taking into account boundary layer have been determined. Measure of the angles at that particles fall and fix on the condensing surface has been found out. Sizes of particles carried away by the flow but not involved in the coating deposition are discovered. It is found out that particle size range of powder material used and plasma flow parameters greatly influence on the angle at which particles fix on the surface. This in turn, essentially effects on the plasma coating structure and its cohesive strength with the constructional materials surface.

1. Introduction

Special coatings to enhance reliability of products under severe external factors are used nowadays. These coatings allow changing physicochemical properties of initial surfaces. Gas-thermal method of coating deposition of powder material is the most common among the variety of methods [1-11,18]. Widely used and economically viable application of plasma gas-thermal method in leading foreign companies is stipulated by the engine engineering, especially by gas turbine production to get heat-protective and thermal-barrier coatings. This method actually replaced various vacuum methods due to a set of advantages [1-2,4].

Main advantages of plasma gas-thermal method are high manufacturability and productivity especially using up-to-date computer-aided design systems CAD/CAE/CAM with robot complexes and possibility to deposit coatings of desired thickness on the complex profiled and internal surfaces. Key features of these coatings are their layer structure and location of crystallite boundaries along the constructional material surface that results in enhancing of high-temperature gas corrosion resistance, oxidation and thermocycling resistance. This structure of plasma coatings fundamentally differs from coating structures manufactured by vacuum electron-beam and ion-plasma methods because their structures have columnar nature. Each separate structure column consists of some crystallites of smaller size perpendicular to the base surface. Boundaries between such crystallites extend from the coating surface up to the base surface. Availability of such vertical boundaries results in formation of canals for penetrating of oxygen ions, harmful impurities and other chemical elements to the protected constructional materials. Besides, vertical column boundaries are stress concentrators, and they result in endurance limit reduction of parts in comparison with the parts without coatings.
Powder materials used for plasma coating deposition regardless of their composition have rather wide size dispersion stipulated by their manufacturing nature. As a result, when powder material particles are brought into the gas flow, they do not move strictly along the flow axis, but along separate trajectories with different angles, speeds and heating temperatures. When falling on the surface of deposition, these disperse particles of powder material with divergent thermal and kinetic state form crystallites of various forms and sizes. Moreover, they have various degrees of deformation because of hit and various cohesive strength with the constructional material surface. Research of this structure using coating cross sections manufactured by some manufactures including foreign ones shows that it consists of disk-shaped clusters having various degree of deformation and slightly deformed spherical particles. Such structure is characterized by wide anisotropy of properties, and it results in the global coating quality is determined by the quality of local structure volumes with minimal values of physical-mechanical properties and operating characteristics.

Understanding of such nature of reduction of coating operating characteristics leads to necessity of complex research to get much more homogeneous and arranged structure. It is possible to achieve this effect due to more detailed research of powder material particles transfer in the plasma flow to the condensation surface and development of manufacturing suggestions based on research results.

2. Statement of mathematical model of disperse particle movement in the plasma flow in the field of boundary layer during plasma spraying

More accurate description of acceleration and transfer processes is impossible without analysis of powder material movement near the surface of deposition and without determination of the angle at which particles fall and fix on the surface of deposition. When modelling powder material particles acceleration and transfer processes, most papers [2-5,7-9,17] do not consider the fact that plasma flow consists of some specific regions, such as core region with constant flow parameters, mixture region and steady flow region where plasma parameters are variable values, and boundary layer region (Figure 1). Besides, it is not considered that particles of different diameters happen in the plasma flow at different times and they move differently. As a result, fine-dispersed particles enter the boundary layer region at essentially different velocity and trajectory. Changing of velocity field of particle mass center and changing of trajectories happen because of flowing above the surface of deposition in the boundary layer region. This results in velocity reduction and even greater trajectory displacement from the flow axis. As a result, particles fall on the surface of deposition at various angles. Fixing of particles on the surface because of unorthogonal hit with slower velocities inevitably results in disordered structure formation consisting of clusters having various degree of plastic deformation with little contact area and short period of pressure action on the contacting surfaces. Strong links cannot be formed during these very short periods. Application of such coating formation mechanism contributes to essential reduction of adhesion and cohesive strength. This fact is not described in most papers. It is assumed [2-5,7-9,16] that the particle independently on its size moves in the flow center and fixes on the product surface due to orthogonal hit. There are no analytical and experimental data on determination of values of angles at which particles fall and fix on the surface of deposition.

Movement of powder material particles in the boundary layer when falling on the surface of deposition is a particular case of particle movement after the plasma flow core. In this case, plasma flow with the particles accumulates on the surface of deposition that can be compared with the wall put across the stream. The stream flows along the obstacle to the opposing sides from some critical point $O$ (Figure 2).

Equations of individual particle motion in the boundary layer region with thickness $\delta$ taking into account accelerating forces along axes $x$ and $y$ applied to the particle mass center according to the deposition scheme (Figure 1) can be represented as:

$$m \frac{dV_x}{dt} = \rho_s C_s \frac{S_m}{2} \left(U_x - V_x\right)^2;$$

$$m \frac{dV_y}{dt} = \rho_s C_s \frac{S_m}{2} \left(U_y - V_y\right)^2;$$
Figure 1. Specific regions of plasma flow: БЕВ1 – core region of plasma flow; CBE и C1B1E – mixture regions; DBЕ и D1B1E – steady flow regions; FDD1F1 – boundary layer region.

Figure 2. Flowing of plasma stream in the region of critical point О.

\[ V(x_\delta) = V_{\delta,x}; \quad V(y_\delta) = V_{\delta,y}; \]  
\[ C_x = \frac{C_{0x}}{Re^k}; \quad C_y = \frac{C_{0y}}{Re^k}, \]  

where \( V_x \) and \( V_y \) – velocity components of particle mass center; \( U_x \) and \( U_y \) – velocity components of gas flow speed; \( m = \pi \rho D^3/6 \) – mass of powder material particle; \( S_m = \pi D^2/4 \) – area of almond-shaped particle section; \( \rho_g \) – gas flow density; \( \rho \) – density of powder material particle; \( D \) – particle diameter; \( C_x \) and \( C_y \) – particle drag coefficient; \( C_{0x}, C_{0y}, k \) – dimensionless parameter of drag; \( Re = (U-V)D/\nu \) – Reynold’s number; \( \nu \) – kinematic viscosity of a gas flow; \( x_\delta \) and \( y_\delta \) – coordinates of particle mass center when it enters into the boundary layer region; \( V_{\delta,x} \) and \( V_{\delta,y} \) – velocity components of particle mass center when it enters into the boundary layer region.
Substituting \( \frac{dV}{dt} = V_x \frac{dV_x}{dx} ; \frac{dV_y}{dt} = V_y \frac{dV_y}{dy} \), we get:

\[
V_x \frac{dV_x}{dx} = B_1 \left( U_x - V_x \right)^{2-k}; \tag{5}
\]

\[
V_y \frac{dV_y}{dy} = B_2 \left( U_y - V_y \right)^{2-k}; \tag{6}
\]

\[
B_1 = \frac{3 \rho C_0 \nu^k}{4 \rho D^{k+1}}; \quad B_2 = \frac{3 \rho C_0 \nu^k}{4 \rho D^{k+1}}. \tag{7}
\]

Considering equation of continuity [13, 14] \( \frac{dU_x}{dx} + \frac{dU_y}{dy} = 0 \) in the region of boundary layer with thickness \( \delta \), equations for the velocity components of potential flowing of plasma flow are the following:

\[
U_x = -ax; \quad U_y = ay; \quad \tag{8}
\]

where \( a = \text{const} \) – velocity gradient of a plasma flow.

Having substitute (8) in (5-6) we get:

\[
V_x \frac{dV_x}{dx} = B_1 \left( -ax - V_x \right)^{2-k}; \tag{9}
\]

\[
V_y \frac{dV_y}{dy} = B_2 \left( ay - V_y \right)^{2-k}. \tag{10}
\]

In the boundary layer region, Reynolds' numbers are of small values. At the same time, particle drag coefficients \( C_x \) and \( C_y \) coincide with theoretical value [14], and they are determined according to the Stokes formula:

\[
C_x = \frac{24}{Re}; \quad C_y = \frac{24}{Re}. \tag{11}
\]

Taking into account Stokes flowing mode (11) equation of movement of an individual particle (9-10) in the boundary layer region can be written as a function of velocity for the corresponding coordinate:

\[
V_x \frac{dV_x}{dx} = -abx - bV_x; \quad V \left( x_\delta \right) = V_{x', \delta}; \tag{12}
\]

\[
V_y \frac{dV_y}{dy} = aby - bV_y; \quad V \left( y_\delta \right) = V_{y', \delta}; \tag{13}
\]

\[
b = \frac{18 \rho \nu^k}{\rho D^{k+1}}. \tag{14}
\]

To determine boundary layer thickness \( \delta \) we use equation for the flowing near the critical point presented in the paper [14]:

\[
\delta = 2.4 \left( \frac{\nu}{a} \right)^{1/2}. \tag{15}
\]

Knowing that in the boundary layer region speed components of potential flowing of plasma flow are proportionate to the coordinate, the following relation is true:

\[
U_x = -ax = -a\delta, \quad \tag{16}
\]

Substituting (16) into (15), we get the relation for velocity gradient of plasma flow:

\[
a = \left( \frac{U_{x, \infty}}{5.76\nu} \right)^2, \tag{17}
\]

where \( U_{x, \infty} \) – velocity of incident plasma flow during transition to the boundary layer region.
In the same manner, we can write the relation for boundary layer thickness on $U_{\infty}$:

$$\delta = \frac{5.76 \nu}{U_{\infty}}.$$  

(18)

3. Mathematical model of disperse particle movement in the plasma flow in the field of boundary layer during plasma spraying

Let us find analytical solution for the velocity component of particle mass center $V_x$ in the boundary layer region. Differential equation (12) is the Abel equation of the second kind. Substituting $V(x) = x \omega(x)$:

$$\omega^2 + x \omega \frac{d\omega}{dx} = -b\omega - ab.$$  

(19)

Having multiplied left and right parts of equation (13) by $\frac{dx}{d\omega}$ and having transformed it, we get

$$\ln |x| = -\int \frac{\omega d\omega}{\omega^2 + b\omega + ab}.$$  

(20)

Having integrated the right part of the equation (20), we can write

$$\int \frac{\omega d\omega}{\omega^2 + b\omega + ab} = 0.5 \ln \left( t^2 + c_i^2 \right) - f_i \cdot \arctg \left( \frac{t}{c_i} \right),$$

(21)

where $t = \omega + 0.5b$; $c_i = \left( ab - 0.25b^2 \right)^{1/2}$; $f_i = \left( \frac{b}{4a - b} \right)^{1/2}$.

When depositing coating of powder material $ZrO_2 - 8\%Y_2O_3$ with dispersion up to $100 \mu m$ at the design modes, parameter $b$ changes within $b = \left[ 27.311 \div 3.933 \cdot 10^5 \right]$, velocity gradient of plasma flow $a = \left[ 849 \cdot 10^4 \div 1086 \cdot 10^4 \right]$. Thus parameter $c_i$ is within the range $c_i = \left[ 1.523 \cdot 10^4 \div 2.057 \cdot 10^6 \right]$, parameter $f_i = \left[ 8.968 \cdot 10^{-4} \div 0.096 \right]$. Taking into account that $t/c_i < 0.2$, to an accuracy at least 1.5 % we can assume $\arctg \left( t/c_i \right) = t/c_i$. Then integral (21) is:

$$\int \frac{\omega d\omega}{\omega^2 + b\omega + ab} = 0.5 \ln \left( t^2 + c_i^2 \right) - k_1t,$$

(22)

where $k_1 = f_i/c_i$.

Having substituted integral solution (22) in the equation (20), we get

$$x^2 \left( t^2 + c_i^2 \right) = \Phi_0^2 \exp \left( 2k_1t \right),$$

(23)

where $\Phi_0 = const$.

Taking into consideration that $2k_1t < 0.1$ and having expanded the function $\exp \left( 2k_1t \right)$ in the Maclaurin series with accuracy loss not exceeding 0.45 % we can claim that $\exp \left( 2k_1t \right) = 1 + 2k_1t$.

According to reasonable assumptions (23):

$$x^2 \left( t^2 + c_i^2 \right) = \Phi_0^2 \left( 1 + 2k_1t \right).$$

(24)

Solving (24) allowing for $t = \omega + \frac{b}{2} = \frac{V}{x} + \frac{b}{2}$ and $V(x_s) = V_{\delta,x}$, we get the relation for determination of movement velocity of particle mass center $V_x$ in the boundary layer region:
Thus, we get analytical solution for the movement velocity component of the particle mass center $V_y$ in the boundary layer region. Differential equation (13) as well as the equation (12) is Abel equation of the second kind. We substitute $V(y) = y \omega(y)$:

$$\omega^2 + y \omega \frac{dy}{d\omega} = ab - b\omega.$$  (27)

Having multiplied left and right parts of the equation (27) by $\frac{dy}{d\omega}$ and having transformed it we get

$$\ln|y| = -\int \frac{\omega d\omega}{\omega^2 + b\omega - ab}. \quad (28)$$

Having integrated right part of the equation (28), we write

$$\int \frac{\omega d\omega}{\omega^2 + b\omega - ab} = \frac{1}{2} \ln\left|\frac{\omega^2 - c_2^2}{\omega^2 - c_2^2 + t}\right| - \ln\left(\frac{c_2 - t}{c_2 + t}\right)^{f_2}.$$  (29)

where $t = \omega + 0.5b$; $c_2 = (ab + 0.25b^2)^{1/2}$; $f_2 = \left(\frac{b}{4a + b}\right)^{1/2}$.

$$\left(\frac{c_2 - t}{c_2 + t}\right)^{f_2} = \left(1 - \frac{t}{c_2}\right)^{f_2} \left(1 + \frac{t}{c_2}\right)^{-f_2}.$$  (30)

Taking into account that $c_2 = \left[1.523 \cdot 10^7 \div 2.076 \cdot 10^6\right]$, parameter $f_2 = \left[8.968 \cdot 10^{-4} \div 0.095\right]$, and also $|t/c_2| < 0.2$; $|-t/c_2| < 0.2$ condition of absolute convergence of series $(1 - t/c_2)^{f_2}$ and $(1 + t/c_2)^{-f_2}$ is complied. In this case, to reach rapid convergence of series to a precision of 0.21% first two terms of series are enough. Thus:

$$\left(\frac{c_2 - t}{c_2 + t}\right)^{f_2} = \left(1 - \frac{t}{c_2}\right)^{f_2} \left(1 + \frac{t}{c_2}\right)^{-f_2} = \left(1 - \frac{f_2 t}{c_2}\right)^2.$$  (31)

With accuracy loss not exceeding 0.04% we can assume

$$\left(\frac{c_2 - t}{c_2 + t}\right)^{f_2} = 1 - 2k_2 t,$$

where $k_2 = f_2/c_2$.

Taking into account performed transformations integral (29) is as follows:

$$\int \frac{\omega d\omega}{\omega^2 + b\omega - ab} = \ln\left|\frac{t^2 - c_2^2}{1 - 2k_2 t}\right|^{1/2}.$$  (32)

Having substituted solution of the integral (30) in the equation (28), we get
\[
\frac{y^2}{\Omega_0} = \frac{1 - 2k_2f}{t^2 - c_2^2},
\]

(31)

where \( \Omega_0 = \text{const} \).

Solving (31) when \( t = \omega + \frac{b}{2} = \frac{V}{y} + \frac{b}{2} \), and \( V(y, \delta) = V_{\delta, y} \), we get the relation to determine movement velocity of particle mass center \( V_y \) in the boundary layer region:

\[
V(y) = \left[ k_2 \frac{y_\delta}{y} \Lambda_{\delta, y} \right]^2 + y_\delta \Lambda_{\delta, y} + c_2^2 y^2 \right]^{-1/2} - k_2 \frac{y_\delta}{y} \Lambda_{\delta, y} - \frac{by}{2};
\]

(32)

\[
\Lambda_{\delta, y} = \frac{c_2^2 y_\delta - \left(V_{\delta, y} + \frac{by}{2}\right)^2}{k_2 \left(2V_{\delta, y} + by_\delta\right) - y_\delta}.
\]

(33)

It is necessary to add boundary condition limiting velocity value \( V(y) \) when falling the surface of deposition to the equation (32). It is required because additional acceleration of particles in given direction is connected with action of transverse force arising when surface is flown by the incident flow:

\[
V_{k, y} \leq \sqrt{\left(V_{\delta, x}\right)^2 + \left(V_{\delta, y}\right)^2 - \left(V_{k, x}\right)^2}.
\]

(34)

Using developed dependencies (25-26) and (32-34), we determine values of velocity components of particle mass center \( \text{ZrO}_2 - 8\%Y_2O_3 \) with diameter 11 \( \mu \text{m} \) falling on the surface of deposition with deposition distance 40 mm (Figure 3, Figure 4).

Figure 3. Changing of velocity component \( V(x) \) of the particle \( \text{ZrO}_2 - 8\%Y_2O_3 \) with diameter 11 \( \mu \text{m} \) in boundary layer region under deposition distance 40 mm: \( V(x1) \) – analytical calculation using formulas (25-26); \( \nu(x1) \) – numerical solution of equation (12).

Figure 4. Changing of velocity component \( V(y) \) of the particle \( \text{ZrO}_2 - 8\%Y_2O_3 \) with diameter 11 \( \mu \text{m} \) in boundary layer region under deposition distance 40 mm: \( V(y1) \) – analytical calculation using formulas (32-34); \( \nu(y1) \) – numerical solution of equation (13) with boundary condition (34).
Knowing values of velocity components of particle mass center after passing boundary layer region it is possible to determine particle fix angle when falling on the surface of deposition:

\[ \gamma = \arctg \left( \frac{V(x_k)}{V(y_k)} \right). \]  

(35)

The experience shows that the particles fixing on the part surface at the angles less than 45° essentially disrupt structural order of the coating and can result in reduction of adhesion and cohesive strength by 15 - 20%.

For the powder coating deposition technology the important issue is to discover particle size \( D_{\text{min}} \) that do not fall on the surface of deposition and that are carried away by the flow. To determine diameters of such particles we assume that \( V(x_k) = 0 \) in (35). Having transformed the equation we get:

\[ D_{\text{min}} = 6 \cdot \sqrt{\frac{\rho g \varphi}{\varphi^2 + 8ax_\delta (V_{\delta,x})^2}} \left[ \frac{\rho^2}{(\varphi^2 + \frac{8ax_\delta (V_{\delta,x})^2}{\psi})^{1/2}} - \frac{\varphi}{\psi} \right] ; \]  

(36)

\[ \varphi = 2a \left( x^2 - x^2_\delta \right) \left( V_{\delta,x} + ax_\delta \right) + 1.5x_\delta \left( V_{\delta,x} \right)^2 ; \]

\[ \psi = x_\delta \left[ a \left( 0.5x^2 + 1.5x^2_\delta \right) + 1.5x_\delta V_{\delta,x} \right]. \]

Equation (36) for determination particle diameters \( D_{\text{min}} \) that do not fall on the surface of deposition and carried away by the flow differs from known conservative evaluations, in particular, from common in the technology of plasma deposition of coatings equation given in [4].

4. Conclusion

Research of acceleration and transportation processes of fine-dispersed particles of deposited powder material in the plasma flow taking into account boundary layer influence has been carried out. Mathematical model of fine-disperse particle motion in a two-phase plasma flow in the field of boundary layer has been developed. Relations to determine trajectories, components of mass center velocity and angles at those particles fall and fix on the surface of deposition have been derived. Dependence of particle incidence angle on the surface of deposition on properties of two-phase plasma flow and powder material characteristics has been found out. Relation for determination particle sizes of powder material carried away by the flow but not involved in coating formation has been developed. Applied use of developed relations has been considered by the example of \( \text{ZrO}_2 - 8\%\text{Y}_2\text{O}_3 \) material used to deposit outer ceramic layer in heat-protective coatings. Analysis of modelling results has shown that particles of different diameters fall on the basis surface at different angles. Essential influence on the angle of incidence becomes apparent with particles having diameter less than 25 - 30 μm. It has been discovered that such particles fall and fix on the basis surface at angles less than 45°and this results in disruption of ordered structure and deterioration of protective properties of the coating, in particular, in reduction adhesive strength of the coating with the surface by 15 – 20 %. It has also been found out that particles with diameter less 10 μm are carried away by the incident flow, and they do not fall on the part surface.

5. References

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