Calculation of residual stresses in plasma spray coatings taking into account the build-up process

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Abstract. Methods of calculation of residual stresses in plasma coatings considering extension process for different cases of substrate attachment that are the most common in deposition practice have been developed. According to the developed methods, analytical calculations and experimental research of residual stresses for the coating composed of 70% Al+30% BN have been done.

1. Introduction

It is well known [1-19] that residual stresses arising during the deposition process are the main reason for coating destruction. It is also known that residual stresses result from non-uniform plastic strain, non-uniform changes of specific volumes during phase transformations, diffusion and chemical reactions, and they result from joining if bodies in the heated state as well.

During the deposition, melted particles hit the substrate at high speed, they are deformed and fixed on the substrate due to the cohesion forces. On crystallization of an individual particle, microscopic stresses arise, they are balanced in the volume of a single particle. However, according to the research, coating strength is determined by the cohesion forces between the particles rather than the material strength of individual particles. Besides, to estimate coating characteristics such notions as modulus of elasticity, heat conductivity coefficient, ultimate stress, etc. are used, but they are averaged for the volumes much greater than the volume of a single particle. In this case, it is possible to consider model continuous process instead of crystallization of individual particles and do calculations based on the available theory of physics of continuous medium.

When considering deposited layer as a continuous medium, macroscopic stresses are of the prime interest because they are balanced in the volume commensurable with the size of the whole sample, that is, they are averaged on the volume much greater than the volume of a single particle. Therefore, when we consider these values, it is reasonably to consider model continuous process instead of crystallization of individual particles. Such model consideration in the framework of the theory of elasticity was first introduced in [19], and then it was further confirmed in the papers [1,2,7]. At the same time, many authors determine the thermal constituent of residual stresses considering wholly formed coating. Practically, residual stresses are formed at the gradual extension of the coating, and on the gradual increase of loads and temperature up to some final value.

Analysis has shown that the final value of residual stresses in coatings calculated subject to the gradual extension of layers essentially differs from the values of residual stresses determined at applying loads and temperatures to the wholly formed coating.

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This article solves the task of determination of residual stresses subject to the gradual extension of the coating with different manners of substrate attachment.

2. Mathematical simulation of residual stresses in plasma coatings subject to the extension process

Let us consider a homogeneous plate (substrate) of thickness \( h \), it is deposited with the material having another thermal-physic and elastic constants that do not depend on the temperature (Figure 1). For the convenience of further calculations, it is assumed that Poisson ratio \( \mu \) of the substrate and the deposited material are the same, and geometrics of the plate is such that state of plane stress is realized, and Kirchhoff hypothesis can be applied. Thus, components of stress \( \sigma_{ix}, \tau_{xy} \), where \( i = x, y \) is distinct from zero.

![Figure 1. Scheme for calculation of residual stresses.](image)

Let the coating of thickness \( \eta \) has been deposited by the given point of time. Temperature distribution through the material thickness \( z \) depending on the mobile boundary \( \eta \) is set up according to [20]. On depositing and setting of the following thin layer as a result of temperature change \( T(z, \eta) \) of all the system, alterations of boundary conditions and moments, the rise of crystallization stresses \( \sigma_{ix}^{(k)}, \tau_{xy}^{(k)} \) in the layer \( d\eta \), stresses inherent in the material will change by the value \( \Delta \sigma_{ix}, \Delta \tau_{xy} \). Crystallization stresses are the stresses naturally distinct from thermos-elastic ones, which is some initial stresses arising when the layer \( d\eta \) is being formed because of the discrepancy of crystal lattices, phase and structural transformations, etc. It is assumed that dependencies \( \sigma_{ix}^{(k)}, \tau_{xy}^{(k)} \) are given. Since on plasma deposition the layer \( d\eta \) is formed from the liquid phase there are only crystallization stresses, and thermos-elastic stresses equal zero.

On successive and continuous forming of the layer with final thickness \( H \), and knowing \( \Delta \sigma_{ix}, \Delta \tau_{xy} \) we get stresses in the layer of final thickness through integration to \( d\eta \). If the material is cooled up to the ambient temperature after deposition finishing, and the attachment device is removed, remaining stresses in the material, namely, residual stresses are determined by the following equations:

\[
\sigma_i(z) = \sigma_i^{(k)}(z) + \int_{z}^{H} \Delta \sigma_i(z, \eta) + \sigma_i^{(b)}(z) \\
(1)
\]

\[
\tau_{xy}(z) = \tau_{xy}^{(k)}(z) + \int_{z}^{H} \Delta \tau_{xy}(z, \eta) + \tau_{xy}^{(b)}(z) \\
(2)
\]
in the substrate \( \sigma_i (z) = \sigma_i^{(n)} (z) + \sum_{n=0}^{\infty} \Delta \sigma_i (z, \eta) - \sigma_i^{(r)} (z) + \sigma_i^{(k)} z , \)

where \( \sigma_i^{(r)} (z) \) – stresses arising on material cooling from final temperature to the ambient temperature; \( \sigma_i^{(k)}, \tau_{xy}^{(k)} \) – stresses arising on removing of attachment device; \( \sigma_i^{(n)} , \tau_{xy}^{(n)} \) – stresses existing in the substrate before deposition. Stresses \( \sigma_i^{(r)} (z) \) can be found from the solution of the thermoelasticity problem.

To determine \( \Delta \sigma_i (z, \eta) \) and \( \Delta \tau_{xy} (z, \eta) \) we use the Kirchhoff hypothesis for plates. Then alteration of shifts \( \Delta u_{ij} \) to distance \( z' \) from the main surface depending on alteration of shifts \( \Delta u_{ij} \) because of layer deposition \( d\eta \) is the following after corresponding transformations and subject to main surface shift:

\[
\Delta u_{ij} (z') = \Delta u_{ij} - z' \frac{\partial \Delta u_{ij}}{\partial z}, \quad \Delta u_{ij} (z') = \Delta u_{ij} + \delta z, \quad \Gamma \delta z \quad i = x, y
\]

and alteration of strain tensor is the following:

\[
\Delta \varepsilon_{ij} (z') = \Delta \varepsilon_{ij} - z' \frac{\partial^2 \Delta u_{ij}}{\partial z^2}, \quad \Delta \gamma_{xy} (z') = \Delta \gamma_{xy} - 2z' \frac{\partial^2 \Delta u_{ij}}{\partial x \partial y}.
\]

Using generalized Hooke law we get an equation for the alteration of strain tensor:

\[
\Delta \sigma_i = \frac{E(\delta')}{1 - \mu^2} \left( \Delta \varepsilon_i + \mu \Delta \varepsilon_j \right) - \frac{E(\delta')}{1 - \mu^2} \delta' \left( \frac{\partial^2 \Delta u_{ij}}{\partial i^2} + \mu \frac{\partial^2 \Delta u_{ij}}{\partial j^2} \right) - E(\delta') \alpha_y(\delta') \frac{\partial \eta}{\partial \delta} d\eta
\]

\[
\Delta \tau_{xy} = \frac{E(\delta')}{2(1 + \mu)} \Delta \gamma_{xy} - \frac{E(\delta')}{2(1 + \mu)} \delta' \frac{\partial^2 \Delta u_{ij}}{\partial x \partial y},
\]

where \( \alpha_y (\delta') \) – coefficient of thermal expansion; \( E(\delta') \) - Young modulus.

Let us introduce, as it is usually done when solving the thermos-elastic task for plates, equivalent forces and moments taken relative to the unit of length. Then alteration of these equivalent forces \( \Delta N_i, \Delta N_{xy} \) and moments \( \Delta M_{ij}, \Delta M_{xy} \) on increasing of plate thickness by \( d\eta \) subject to crystallization stresses in the layer \( d\eta \) is connected with alteration of stresses on this layer using the following relations:

\[
\Delta N_i = \int_{-\delta(\eta)}^{\delta(\eta)} \Delta \sigma_i z' + \sigma_i^{(k)} (\eta) d\eta; \quad \Delta M_{ij} = \int_{-\delta(\eta)}^{\delta(\eta)} \Delta \sigma_i z' \delta z' + \sigma_i^{(k)} (\eta) g (\eta) d\eta
\]

where \( \delta (\eta) \) and \( g (\eta) \) – distances from the main surface to the lower and upper surfaces of the deposited plate. Relations for \( \Delta N_{xy}, \Delta M_{xy} \) are developed the same way.

Applying (5) and (6) to (7) and using the definition of the main surface, we get:

\[
\Delta N_i = \frac{A(\eta)}{1 - \mu^2} \left( \Delta \varepsilon_i + \mu \Delta \varepsilon_j - (1 + \mu) \Delta \varepsilon_t \right) + \Delta \sigma_i^{(k)} (\eta) d\eta
\]

\[
\Delta N_{xy} = \frac{A(\eta)}{2(1 + \mu)} \Delta \gamma_{xy} + \tau_{xy}^{(k)} (\eta) d\eta
\]

\[
\Delta M_{ij} = \frac{D(\eta)}{1 - \mu^2} \left( \frac{\partial^2 \Delta u_{ij}}{\partial i^2} + \mu \frac{\partial^2 \Delta u_{ij}}{\partial j^2} \right) + (1 + \mu) \Delta \chi_{ij} \right) + \sigma_i^{(k)} (\eta) g (\eta) d\eta
\]

\[
\Delta M_{xy} = - \frac{D(\eta)}{1 + \mu} \frac{\partial^2 \Delta u_{ij}}{\partial x \partial y} + \tau_{xy}^{(k)} (\eta) g (\eta) d\eta
\]
\[
A(\eta) = \int_{-\delta(\eta)}^{\delta(\eta)} E(z')dz'; \quad D(\eta) = \int_{-\delta(\eta)}^{\delta(\eta)} E(z')(z')^2dz',
\]

where \(A(\eta), A(\eta)\) – tension and bending stiffness of the plate.

\[
\Delta e_x = \frac{1}{A(\eta)} \left[ \int_{-\delta(\eta)}^{\delta(\eta)} E(z')\frac{\partial^2 T}{\partial \eta} dz' \right] d\eta
\]

\[
\Delta \chi_x = \frac{1}{D(\eta)} \left[ \int_{-\delta(\eta)}^{\delta(\eta)} E(z')\frac{\partial T}{\partial \eta} dz' \right] d\eta
\]

(10)

Using the equations (5), (6), (8) and (9) we get:

\[
\Delta \sigma_i = \frac{E(z')}{A(\eta)} \left[ \Delta N_i - \sigma_i^{(i)}(\eta) d\eta \right] + z' \frac{E(z')}{D(\eta)} \left[ \Delta M_i - \sigma_i^{(i)}(\eta) g(\eta) d\eta \right] +
\]

\[
+ \frac{E(z')}{1 - \mu} \left[ \Delta e_x + z' \Delta \chi_x + \alpha_x(z') \frac{\partial T}{\partial \eta} d\eta \right]
\]

(11)

\[
\Delta \tau_{xy} = \frac{E(z')}{A(\eta)} \left[ \Delta N_{xy} - \tau_{xy}^{(i)}(\eta) d\eta \right] + z' \frac{E(z')}{D(\eta)} \left[ \Delta M_{xy} - \tau_{xy}^{(i)}(\eta) g(\eta) d\eta \right]
\]

(12)

Based on well-known assumptions that residual stresses are constant over the coating length out of the edge effect region (dimensions of edge effect are comparable with the substrate and coating height), let us consider the most common events of substrate attachment used in deposition practice.

3. Residual stresses in the plate free from boundary forces and moments

Taking into account that \(\Delta N_i = \Delta N_{xy} = 0; \Delta M_i = \Delta M_{xy} = 0\), we get:

\[
\Delta \sigma_i = -E(z') \left[ \frac{1}{A(\eta)} + z' \frac{g(\eta)}{D(\eta)} \right] \sigma_i^{(i)}(\eta) d\eta +
\]

\[
+ \frac{E(z')}{1 - \mu} \left[ \Delta e_x + z' \Delta \chi_x - \alpha_x(z') \frac{\partial T}{\partial \eta} d\eta \right]
\]

(13)

\[
\Delta \tau_{xy} = -E(z') \left[ \frac{1}{A(\eta)} + z' \frac{g(\eta)}{D(\eta)} \right] \tau_{xy}^{(i)}(\eta) d\eta
\]

(14)

Thermal stresses on the cooling of the already formed plate are:

\[
\sigma_i = \frac{E(z')}{1 - \mu} \left[ \frac{1}{A(H)} \int_{-\delta(H)}^{\delta(H)} \alpha_x(z')E(z')T(z',H)dz' +
\right.

\[
+ \frac{z'}{D(H)} \int_{-\delta(H)}^{\delta(H)} \alpha_x(z')E(z')z'T(z',H)dz' - \alpha_x(z')T(z',H)
\]

(15)

Having substituted (14), (13) and (15) into (1-4), we get the formula for calculation of residual stresses in the system after deposition.

4. Residual stresses in the fully constrained plate

Full constraint means such a joint of the plate that excludes any substrate strain. In this case, from (8) and (9) we get that under deposition alteration of contour forces and moment will be the following:
\[ \Delta M_i = - \frac{D(\eta)}{1 - \mu} \Delta X_i + \sigma_{\alpha}^{(i)}(\eta) g(\eta) d\eta; \quad \Delta M_{xy} = \tau_{\alpha xy}^{(i)}(\eta) g(\eta) d\eta \quad (16) \]

\[ \Delta N_i = - \frac{A(\eta)}{1 - \mu} \Delta e_x + \sigma_x^{(i)}(\eta) d\eta; \quad \Delta N_{xy} = \tau_{\alpha xy}^{(i)}(\eta) d\eta \quad (17) \]

\[ \Delta \sigma_i = - \frac{E(z')\alpha_x(z') \frac{\partial T}{\partial \eta}}{1 - \mu} d\eta; \quad \Delta \tau_{xy} = 0 \quad (18) \]

On completion of the process of forming the deposited layer and removing the fasteners from the plate, the forces and moments are applied to the plate boundary that determined from equations (16) and (17) with the reversed sign:

\[ M_i = \int_0^H \left[ \frac{D(\eta)}{1 - \mu} \Delta X_i - \sigma_{\alpha}^{(i)}(\eta) g(\eta) d\eta \right] d\eta; \quad M_{xy} = - \int_0^H \tau_{\alpha xy}^{(i)}(\eta) g(\eta) d\eta \quad (19) \]

\[ N_i = \int_0^H \left[ \frac{A(\eta)}{1 - \mu} \Delta e_x - \sigma_x^{(i)}(\eta) d\eta \right] d\eta; \quad N_{xy} = - \int_0^H \tau_{\alpha xy}^{(i)}(\eta) d\eta \quad (20) \]

Stresses arising because of applying forces and moments in the plate are the following:

\[ \sigma_{\alpha}^{(i)} = \frac{E(z')N_i}{A(H)} + z' \frac{E(z')M_i}{D(H)}; \quad \tau_{\alpha xy}^{(i)} = \frac{E(z')N_{xy}}{A(H)} + z' \frac{E(z')M_{xy}}{D(H)} \quad (21) \]

Having substituted (18), (21) and (14) into (1-4), we get the design formula for residual stresses in the fully constrained plate.

5. Residual stresses in the partially constrained plate

Partially constrained attachment is such a joint that provides free stretching or compression of the plate, but restricting its bend, that is \( \Delta N_i = \Delta N_{xy} = 0; \Delta u_x = 0 \).

Alteration of contour moment on deposition is determined by the expression (16), and stress alteration will be the following:

\[ \Delta \sigma_i = - \frac{E(z')}{A(\eta)} \sigma_{\alpha}^{(i)}(\eta) d\eta + \frac{E(z')}{1 - \mu} \left[ \Delta e_x - \alpha_x(z') \frac{\partial T}{\partial \eta} d\eta \right] \quad (22) \]

\[ \Delta \tau_{xy} = - \frac{E(z')}{A(\eta)} \tau_{\alpha xy}^{(i)}(\eta) d\eta \]

After releasing of the plate, the following stresses arise:

\[ \sigma_{\alpha}^{(i)} = z' \frac{E(z')M_i}{D(H)}; \quad \tau_{\alpha xy}^{(i)} = z' \frac{E(z')M_{xy}}{D(H)} \quad (23) \]

where \( M_i \) and \( M_{xy} \) are determined according to (19).

Having substituted (22), (23) and (14) into (1-4), we get calculation formula for residual stresses in a partially constrained plate.

6. Results and discussion

To approve this method theoretical calculations and experimental research of residual stresses in the samples under the same deposition conditions have been done (Figure 2).

Samples for research were thin plates with dimensions 100x10x2.5 mm and the deposited layer of 70% Al+30% BN. Sample strain was measured during continuous electropolishing. For the etching of the layer, 70% Al+30% BN 15% solution of KOH was used. To provide a constant rate of sample electropolishing they were impregnated with a specific oil and the current was stabilized.
Figure 2. Residual stress diagram depending on the attachment of the substrate (deposition of 70% Al+30% BN on steel): a – rigid attachment; ○ – experimental data, × – analytical calculation; b – free attachment: Δ – experimental data, • – analytical calculation.

7. Conclusion
Method of determining residual stresses in deposited coatings for main condition attachments of substrates that are the most common in deposition practice has been developed. Application of this method has been shown by the example of the determination of residual stresses in the deposited coating of 70% Al+30% BN. Figure 2 displays the results of residual stresses obtained by means of theoretical calculations and experimental research. Results have shown that residual stress diagrams obtained theoretically display good convergence with the experiment.

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