The numerical optimization methods usage for choosing blisk trajectory during PVD coating deposition

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Abstract. PVD coating deposition is a considerable way to prevent the gas turbine engine blade from erosive wear. However, the process for blisks is complicated by the part complex shape which leads to uneven film thickness. The research considers an approach for optimizing the blisk trajectory in a vacuum chamber. This approach reduced the calculated non-uniformity of the coating thickness from $4.3 \times 10^{-8}$ to $6.2 \times 10^{-4} \mu m$.

1. Introduction

The gas turbine engine performance improvement is one of the most important scopes in keeping aviation technology competitive [1]. This race led to the development of an integrated disc and blade design called blisk, which allows to increase specific compressor parameters.

During the operation process, blisk blades face a wide range of effects from dynamic stresses in a various temperature of the gas flow containing abrasive particles, oxidized products from the environment and from fuel combustion, etc. [2]. Finishing is one of the effective ways to ensure the blade resource. Today the only method of blisk blades hardening entered into mass production is conventional shot peening, which creates compressive stresses in the surface and, as a result, increases the part’s fatigue endurance limit [1, 3]. However, the issue of protecting blisk from erosive wear remains unresolved and PVD coating deposition is the most promising method for dealing with it [4].

Technologies for single blades processing exist and show acceptable results [5], however, the most common method of blisk forming is milling from a non-profiled workpiece [6]. This means that the entire set of blades need to be coated at a single deposition process. The complex geometry of the part creates areas of optical shadow in the particles movement path due to land-of-sight problem [7], which leads to the uneven processing and, as a result, the nonuniform coating thickness. The classic way to reduce this influence is performing complex movement of the part in a vacuum chamber during processing [7]. Experimental trajectory selection would require significant material and time costs, which can be reduced using numerical modeling and optimization methods. In this paper, an approach to the part’s motion law selection during PVD coating deposition is considered.

2. Calculations

Despite the complexity of the occurring plasma processes, there are numerous models for coating thickness calculation. They are useful for obtaining preliminary recommendations for the deposition process and chamber elements design.
Since plasma is a quasi-neutral ionized gas, the CFD approach is fertile. To proceed the coating thicknesses calculation, it is necessary to add equations for particle motion to the laws describing the gas flow in the chamber. Then, based on their trajectories, the weight gain on the substrate is calculated and, as a consequence, the thickness of the coating. For example, in [8, 9], the Eulerian wall film model of the Ansys Fluent software package was used to get the film thickness distribution without taking into account electrical and magnetic forces. Another successful approach is the Monte Carlo method. It allows to predict not only the thickness distribution, but also the coating structure. The first step is to calculate the number of particles flying up to the substrate, and then determine their behavior when colliding with the substrate. A single particle may bounce off, settle onto the part, or evaporate according to the probability of each outcome [10]. The models described in [11, 12, 13, 14] use a combination of the CFD model with the Monte Carlo method, which showed the coating columnar structure.

The described models work, however, unfortunately, these approaches show satisfactory results for relatively high pressures (> 1 and even 100 Pa). This is due to the fact that the Knudsen number for low and high vacuum, is greater than 0.1, which means that the gas flows not in a continuum, but in a transition or molecular regime, and collisions with the chamber walls prevail over intermolecular ones. To describe the processes occurring at 10^3 Pa, it is necessary to use completely different approaches. Such models are based on the laws of geometry.

The mass gain and, as a result, the coating growth, is the function of the distance r between the center of the substrate element and the vapor source, the angle ψ between the direction of the emitted atom and the symmetry of the evaporation source, angle Θ between the normal to the surface at the center of the substrate element with area dA and the incident vapor source beam. This approach showed acceptable results for fixed [16, 17] and moving [18, 19, 20, 21] surfaces.

Shown above models were developed by the authors independently using delphi or Matlab and show satisfactory convergence with experimental results. However, if it is necessary to calculate details of a complex shape, expressed in the presence of optical shadow areas on the path of the coating particles, which are, for example, blisks or set of stator blades, a complex kernel will be required to take into account the effects associated with shading, which can be avoided using ready-made software packages, for example, COMSOL Multiphysics.

The developed model is based on the following provisions:

- Sputtered particles of the cathode material move along linear trajectories without interacting with particles of the reaction gas. Under vacuum conditions (10^2 Pa) the free path of an ion is comparable to the size of the chamber, and weak magnetic fields are not distort the trajectory of ions [22].
- Particles condense directly at the point of impact with the substrate surface. This means that the diffuse movement of particles over the substrate surface is not taken into account. These displacements are less than a few microns [23], which is incomparable with the dimensions of the products under consideration (tens of millimeters), so they can be neglected.
- Each point of the cathode is equally likely to be a source of charged particles. Ion sources are cathode spots rapidly moving along the cathode surface, which size is in the range of 10^{-2} - 10^{-4} cm. However, taking into account the time scales of the process and the fact that the speed of spots can reach hundreds of meters per second [24], it is reasonable to consider any point of the cathode surface as an equiprobable source of ions.
- The angular distribution of the ion flux density from the cathode obeys the Lambert-Knudsen distribution.

Generally, the calculation of the coating thickness distribution consists of the following stages: geometry building, boundary conditions determination and mesh building. This is followed by calculation and results viewing with a postprocessor.
The geometry of the blisk blades was built using profile objects in the work plane with Loft operation, after that a vacuum chamber was added with ion sources. The final view of the design geometry is shown in figure 1.

![Figure 1. The geometry (Marks are given in the text).](image)

The next step is to determine the boundary conditions (BC). Number 2 marks the boundary between the fixed and rotating interfaces and the Particle Continuity BC in the Mathematical Particle Tracing module. Rotation about the horizontal axis of the blisk is added by specifying the Prescribed Displacement volume condition of the Deformed mesh module using the formula:

\[
\begin{align*}
    d(z) &= (X_g - X_0) \cos(\omega \times t) - (Z_g - Z_0) \sin(\omega \times t) + Z_0 - Z_g \\
    d(x) &= (X_g - X_0) \sin(\omega \times t) + (Z_g - Z_0) \cos(\omega \times t) + X_0 - X_g
\end{align*}
\]

where \(d(z), d(x)\) are the mesh deformations in the z and x-axes, respectively, \(X_g, Z_g\) are the coordinates of the initial position of the system, \(Z_0, X_0\) are the coordinates of the rotation axis, \(\omega\) is the rotation speed, \(t\) is the time.

The addition of the second axis of rotation was simulated by alternately turning on and off the ion sources, which were copied along the outer surface of the chamber (Inlet boundary condition, number 5). This process is demonstrated by the arrows in figure 2, where the first one of the four sources works, then the next while previous are inactive. Thus, the alternate activation and deactivation of 10 Inlets, each consists of four evaporator surfaces, creates the effect of rotation of the blisk in the vertical axis of the chamber, and the change in the angular velocity is regulated by the change in the active state time of each of the four sources. Further, the notion of a particle source will refer to each of the 10 BC Inlet, including 4 surface-inlets.
Boundary conditions on surfaces 3 and 4 - Wall with the Disappear condition.

The control of the coating thickness will be measured along the middle blade surface (number 1 in figure 1), so it has Accumulator Wall BC. As a result of the calculation, the total number of particles per unit surface is calculated. The value of the coating thickness is determined by the formula

\[
\frac{dh}{dt} = \frac{1}{\rho} \frac{dm}{dSdt},
\]

where \( \rho \) is the density of the coating material, \( S \) is the area. To convert the concentration of particles into the thickness of the coating, we transform the formula (1) to the form (2), taking into account that \( m = N \cdot m_1 \), where \( N \) is the number of deposited particles per unit surface, and \( m_1 \) is the mass of each particle:

\[
K_e \cdot c = h,
\]

where \( K_e \) is the empirical coefficient selected in the calculation process. In this case, \( c_{tot} \) is the sum of the concentrations \( c_i \) of each of the ten sources:

\[
c_{tot} = \sum_{i=1}^{10} c_i,
\]

\( c_i \), on the other hand, linearly depends on the total number of particles \( N_i \) emitted during the active period of the source \( t_i \):

\[
c_i = b_i N_i,
\]

where \( b_i \) is a linear coefficient. \( N_i \) linearly depends on the time of active operation of the source \( t_i \) and the number of emitted particles per unit time \( n_i \) . Thus, formula 2 for calculating the thickness of the coating \( h \) at a point is converted to the form:

\[
h = \sum_{i=1}^{10} b_i n_i t_i,
\]

where \( t_i \) is constant for all sources to simplify the calculation process. Thus, the change in processing conditions (rotation speed in the vertical axis) is carried out by varying the parameter \( n_i \).

After specifying the boundary conditions, it is necessary to set up the mesh. It was built automatically with the Fine size of the element. No solver settings were changed, so the standard Iterative is used.
The efficiency of the approach is demonstrated recently [25]. Despite the quantitative differences at some points, the coincidence of the general shape of the curve allows the parameter selection for their optimization.

Blisk trajectory in the vacuum chamber optimization is the main goal of this paper. The optimization criterion is the uniformity of the coating thickness, which, within the framework of the model representation, is found using dependence (5), in which \( n_i \) is the controlled parameter. Thus, it is possible to set the problem of selecting the number of emitted particles \( n_i \) per unit time such that the difference in thickness of the applied coating is minimal.

The solution to this problem was carried out using the COMSOL Multiphysics optimization module. The Optimization Module is an add-on package that can be used with any of the existing COMSOL Multiphysics modules. It is a common interface for setting objective functions, control variables, and constraints.

Working with the module is carried out in 4 stages. First of all, the objective function is determined - a criterion that describes the quality of the system. Then a set of control variables is determined - the initial data of the model that needs to be changed. After that, a set of restrictions and limitation values of control variables is determined. Finally, the Optimization module is applied to improve the results by modifying control variables within specified constraints.

At the first stage, 9 points were selected on the pressure and suction sides of the blade, three in the upper and lower part and in the middle (figure 3). The objective function is the standard deviation \( \sigma \) of the coating thickness at the selected points:

\[
\sigma = \left( \frac{1}{n} \sum_{i=1}^{n} (\bar{h} - h_i)^2 \right)^{\frac{1}{2}},
\]

where \( n = 18 \) is the total number of points for calculation, \( h_i \) - the thickness of the coating at each point, \( \bar{h} \) is the mean thickness of the coating.

To calculate \( \bar{h} \), it is necessary to find the linear coefficients \( b_i \) for each of 18 points (figure 4.6) from 10 sources. For this, a series of 12 calculations was carried out - when only one of ten sources is active (the first, second, and so on up to 10) and 2 test ones, when all are active, and when none are active.

These numbers are linear coefficients in formula (5). Thus, we can write the following system of equations for calculating the objective function:
As a result of the calculation, the value of the target parameter of the standard deviation of the coating is calculated by the formula:

\[ h_1 = 3.2n_1 + 1.3n_2 + 1n_3 + 4.21n_4 + 1.09n_5 + 0n_6 + 0.21n_7 + 0.62n_8 + 0n_9 + 0.44n_{10} \]
\[ h_2 = 4.1n_1 + 1.8n_2 + 0.92n_3 + 3.3n_4 + 1.17n_5 + 0.73n_6 + 0.65n_7 + 0.87n_8 + 0.83n_9 + 0.44n_{10} \]
\[ h_3 = 3.31n_1 + 4.79n_2 + 4n_3 + 3.32n_4 + 3.17n_5 + 1.06n_6 + 0.91n_7 + 1.17n_8 + 1.16n_9 + 3.06n_{10} \]
\[ h_4 = 2.07n_1 + 1.67n_2 + 2.16n_3 + 2.76n_4 + 0.22n_5 + 0n_6 + 0.35n_7 + 0.88n_8 + 0n_9 + 0.33n_{10} \]
\[ h_5 = 2.45n_1 + 1.29n_2 + 1.64n_3 + 2.64n_4 + 0.5n_5 + 0n_6 + 0.76n_7 + 0.65n_8 + 1.76n_9 + 1.05n_{10} \]
\[ h_6 = 3.67n_1 + 5.9n_2 + 5.64n_3 + 3.9n_4 + 2.56n_5 + 1.98n_6 + 0.96n_7 + 0.89n_8 + 1.9n_9 + 2.33n_{10} \]
\[ h_7 = 1.35n_1 + 2.09n_2 + 2.5n_3 + 2.3n_4 + 1.07n_5 + 1.06n_6 + 0.09n_7 + 0.58n_8 + 0.2n_9 + 1.57n_{10} \]
\[ h_8 = 2.52n_1 + 1.81n_2 + 3.6n_3 + 2.94n_4 + 2.5n_5 + 1.8n_6 + 0.02n_7 + 0.05n_8 + 0.69n_9 + 1.67n_{10} \]
\[ h_9 = 1.64n_1 + 3.42n_2 + 5.61n_3 + 3.05n_4 + 3n_5 + 1.38n_6 + 0n_7 + 0.38n_8 + 1.05n_9 + 3.61n_{10} \]
\[ h_{10} = 1.28n_1 + 0.48n_2 + 0.4n_3 + 0.59n_4 + 1.1n_5 + 4.99n_6 + 4.81n_7 + 3.79n_8 + 3.62n_9 + 1.9n_{10} \]
\[ h_{11} = 0.92n_1 + 0.45n_2 + 0.24n_3 + 0.7n_4 + 1.16n_5 + 3.3n_6 + 0.84n_7 + 1n_8 + 3.83n_9 + 0.35n_{10} \]
\[ h_{12} = 0.26n_1 + 0.36n_2 + 0.84n_3 + 0.2n_4 + 3.18n_5 + 2.29n_6 + 0.58n_7 + 0.4n_8 + 1.91n_9 + 0.6n_{10} \]
\[ h_{13} = 1.97n_1 + 0.89n_2 + 0.92n_3 + 1.43n_4 + 0.22n_5 + 4n_6 + 4.64n_7 + 5.72n_8 + 2.71n_9 + 2.6n_{10} \]
\[ h_{14} = 0.56n_1 + 0.7n_2 + 0.35n_3 + 0.81n_4 + 0.5n_5 + 2.36n_6 + 1n_7 + 1.25n_8 + 3.55n_9 + 0.07n_{10} \]
\[ h_{15} = 0n_1 + 0.27n_2 + 0.09n_3 + 0n_4 + 2.55n_5 + 1.84n_6 + 0.88n_7 + 0.95n_8 + 1.88n_9 + 0n_{10} \]
\[ h_{16} = 1.69n_1 + 0.9n_2 + 0.62n_3 + 2.14n_4 + 1.05n_5 + 2.7n_6 + 5.67n_7 + 4.06n_8 + 1.79n_9 + 3.1n_{10} \]
\[ h_{17} = 0.04n_1 + 0.05n_2 + 0n_3 + 0.4n_4 + 2.45n_5 + 1.37n_6 + 1.36n_7 + 1.92n_8 + 2.05n_9 + 0.17n_{10} \]
\[ h_{18} = 0.2n_1 + 0n_2 + 0n_3 + 0.18n_4 + 3.01n_5 + 1.25n_6 + 3.78n_7 + 2.15n_8 + 3.16n_9 + 1.25n_{10} \]

\[
\bar{h} = \frac{1}{8} \sum_{i=1}^{18} h_i
\]

\[
\sigma = \left( \frac{1}{n_{\text{const}}} \sum_{i=1}^{18} (\bar{h} - h_i)^2 \right)^{\frac{1}{2}}
\]  

(8)  

The objective function S is defined. The next step is to define the control variables. By the problem specification, they are \( n_1, n_2, n_3, n_4, n_5, n_6, n_7, n_8, n_9, n_{10} \) - the number of emitted particles per unit time from the source.

At the next stage, as a constraint, a condition for the constancy of the total number of particles was added by the formula:

\[
\sum_{i=1}^{10} n_i = \text{const},
\]  

(9)  

The last step is to add the Optimization module and select an optimization approach. The COBYLA method was selected for the calculation.

When determining the input parameters for the Optimization module, in addition to the above data, the minimum step size was determined, which is assumed to be 0.5 and the maximum number of steps is 1.000.000. The calculation was carried out in order to find the minimum of the objective function.

3. Results and discussion

As a result of the calculation, the value of the target parameter of the standard deviation of the coating thickness has been reduced from 12.7 to 8.8 units. The found values of the design variables are presented in table 1.
Table 1. Calculated values of control variables.

|   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|
| $n_1$ | $n_2$ | $n_3$ | $n_4$ | $n_5$ | $n_6$ | $n_7$ | $n_8$ | $n_9$ | $n_{10}$ |
| 3.3 | 3.3 | 3.3 | 30 | 10.9 | 4.2 | 3.3 | 3.3 | 30 | 3.3 |

The results of calculating the coating thickness after optimization are presented in figures 4 and 5.

As can be seen from figures 4 and 5, the optimization of the rotation speed in the vertical axis of the chamber made it possible to significantly reduce the calculated difference in the thickness of the coating along the blade surface. The range of values before the optimization is $4.3 - 10.8 \, \mu m$, while after it is $6.2 - 10.4$.

To convert the coefficients $n_i$ into the speed of vertical rotation in the camera axis, we transform the already used ratio into the formula:
\[ N_i = n_i \cdot t = k_i \cdot n \cdot t = n \cdot t_i, \quad (10) \]

where \( t_i \) is the time of passage of the \( i \)-th angular step, \( k_i \) is the proportionality coefficient. Thus, we obtain the following formula (4.8) for 10 angular steps \( \varphi_0 = 360°/10 = 36° \) each:

\[ \omega_i = \frac{\varphi_0}{t_i} = \frac{\omega_0 t_i}{k_i t_i} = \frac{\omega_0}{k_i}, \quad (11) \]

where \( \omega_0 \) is the maximum speed of the mechanism. The graph of the change in the obtained angular velocity is shown in figure 6.

**Figure 6.** Graph of changes in angular velocity depending on the angle of rotation of the blisk.

Based on graph 6, it follows that to ensure the uniformity of the applied erosion-resistant PVD coating, it is necessary to reduce the angular velocity of rotation in the vertical axis of the chamber by up to six times compared to its initial value in the range of angles 108-216 degrees. This is due to the fact that, the zones in the root part of the blade is processed at these angles relative to the source, which remain "in the shadow” in the other ranges of angles.

### 4. Conclusion

Thus, the calculations made it possible to choose the function of the angular velocity of rotation of the blisk in the vertical axis of the camera from the angle of its rotation \( \omega_i = f(\varphi) \), which ensures the minimum unevenness of the thickness of the first stage LPC blisk blades PVD coating. The dependence obtained using the developed algorithm is loaded into the stepper motor controller responsible for the rotation of the part in the vertical axis of the chamber, which will reduce the unevenness of the coating thickness.

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