Multi objective optimization of wear resistant TiAlN and TiN coatings deposite by PVD techniques

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ABSTRACT

Purpose: The goal of this paper is to determine, the optimal layer thickness of deposited coatings, in respect of thermal strain and stresses.

Design/methodology/approach: For physical modelling purposes Cr, TiN and TiAlN layers were treated as a continuous medium, so the physical phenomena, occurring in the coating, are modelled based on a classical theory of stiffness. Computer model of the object (coating + substrate) describing strains and thermal stresses states in layers, after deposition process, was created using FEM method.

Findings: The decisional objectives, based on various stresses fields in deposited coating, were defined. The set of optimal TiAlN and TiN layer thickness, in respect to created decision objectives was determined. Also method of optimal solutions set analysis, based on multidimensional, Euclidean metric was created.

Research limitations/implications: There is a need to consider creation of a certain class of selection functions, as a standard, which will help to choose the optimal set of solutions - obtained in different multi objective optimization procedures. Of course, new and more detailed physical and mathematical models of the PVD processes are required.

Practical implications: Proposed multi objective optimization procedure will become a component of the PC software in future, which will make design process of hard, wear resistant coatings architecture possible.

Originality/value: Insertion of the base layer, below TiAlN and TiN tiers, was proposed, whose occurrence is reflected by the continuous change of the physical and chemical properties, across the coating thickness. Also method of optimal solutions set analysis, based on multidimensional, Euclidean metric was created.

Keywords: Computational material science; Thermal stresses; FEM; Multi-objective optimization

Reference to this paper should be given in the following way:
1. Introduction

Optimization of the design process of wear resistant coatings architecture for wood machining tools is nowadays a subject of interest of many research and industrial centres [1-4]. Special interest is paid to coatings deposition processes by PVD technique. Scientific research is focused on multilayer coatings, which may be very effective for improving: adhesion, hardness and fracture toughness resistance. Designing of optimal multilayer coating structure, needs fundamental knowledge about stress/strain profiles - created inside of multilayer coating. The commonly applied Finite Element Method (FEM) provides significant support, for stress/strain profiles, being mainly used for mechanical failure investigations in mono-, duplex- and multilayer coatings. There is a series of publications, related with technological and theoretical aspects of hard, wear resistance coatings deposition [5-10], however only few publications, related to optimal coating (characterized with functionality improvement) architecture prediction were appeared so far. The multi objective optimization of TiN and TiAlN (components of multilayer coating) layers thickness, with respect to thermal strain and stresses, resulting from layer deposition process, is presented in this paper. Presence of the metal Cr base layer, between the substrate and a coating, reducing stresses significantly was also taken into consideration in the optimization procedure. Proposed procedure is using the physical layer model based on FEM.

1.1. Physical model

The modelled objects are hard, wear resistant coatings composed of Ti nitrides (TiN or TiAlN) and Cr layers, deposited on substrate from high speed steel (HSS). The architecture of modelled object is presented in Figure 1. The goal of this modelling process is to determine field of thermal strains and stresses, present in coating layers after deposition with PVD method. The following assumptions, concerning the object, were taken into account during model creation:

- Cr, TiN and TiAlN layers are treated as continuous media,
- the substrate with the multilayer coating is the elastic body,
- there is a perfect adhesion between the substrate and the Cr base layer, and there is a perfect cohesion between layers inside the coating,
- the particular coatings layers have different material properties (Young’s modulus, Poisson’s ratio, thermal expansion coefficient, density),
- coating cooling, after its deposition, was fully radiation process,
- because of the object symmetry: the two dimensional strain, and three dimensional stress states were assumed.

1.2. Mathematical model

Stress state is a symmetric, second-order tensor, with six different components [11-14]. One may transform this tensor to six component vector of the form:

\[
\boldsymbol{\sigma} = \begin{bmatrix} \sigma_x & \sigma_y & \sigma_z & \tau_{xy} & \tau_{xz} & \tau_{yz} \end{bmatrix}^T
\]  

(1)

where:
\[
\sigma_x, \sigma_y, \sigma_z - \text{normal stress along } x, y, z \text{ axes, respectively},
\tau_{xy}, \tau_{xz}, \tau_{yz} - \text{shear stress along } xy, yz, xz \text{ planes, respectively}.
\]

Also tensor which describes the strain state, may be transformed to six component vector. The form of that vector is analogous to the form of vector (1):

\[
\boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon_x & \varepsilon_y & \varepsilon_z & \varepsilon_{xy} & \varepsilon_{xz} & \varepsilon_{yz} \end{bmatrix}^T
\]  

(2)

where:
\[
\varepsilon_x, \varepsilon_y, \varepsilon_z - \text{normal strain (strain of edges of the analysed element), along } x, y, z \text{ axes, respectively},
\varepsilon_{xy}, \varepsilon_{xz}, \varepsilon_{yz} - \text{shear strain, describing angle change, between walls of analysed element}.
\]

Thermal strain is defined by the vector:

\[
\varepsilon^{th} = \Delta T \begin{bmatrix} \alpha_x & \alpha_y & \alpha_z & 0 & 0 & 0 \end{bmatrix}^T
\]  

(3)

where:
\[
\alpha_x, \alpha_y, \alpha_z - \text{thermal expansion coefficients, along } x, y, z \text{ axes, respectively},
\Delta T = T-T_{ref} - \text{temperature increment},
T_{ref} - \text{reference temperature}.
\]

Generalized Hook’s law is given by a formula:

\[
\boldsymbol{\sigma} = D \varepsilon^{th}
\]  

(4)

where:
\[
D - \text{stiffness matrix containing: Young’s and Kirchhoff’s modulus and Poisson’s ratios [11-14].}
\]

Knowing the form of \( \sigma \) vector, Huber Von Mises stresses values, can be calculated with the formula:

\[
\sigma_v = \frac{1}{2} \left[ \left( \sigma_x - \sigma_y \right)^2 + \left( \sigma_y - \sigma_z \right)^2 + \left( \sigma_z - \sigma_x \right)^2 + 6 \left( \sigma_{xy}^2 + \sigma_{xz}^2 + \sigma_{yz}^2 \right) \right]^{0.5}
\]  

(5)

1.3. Computer model

Computer model of the object was implemented in COMSOL Multiphysics environment. The dimensioned model of the object, restraints and a plot of discretization mesh, is presented in Figure 1. Decision variables in this model are layers thickness values:
\[
d_1 \in [0.2 \text{ – } 3] \ \mu m, \quad d_2 \in [0.2 \text{ – } 3] \ \mu m
\]

Fixed dimensions of the modelled object elements are as follows: \( d_3 = 0.5 \ \mu m \), \( d_4 = 15 \ \mu m \) and \( d_5 = 15 \ \mu m \). The remaining physical values, which were used in numerical simulation, are presented in Table 1.
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Fig. 1. The schema of the modelled object with its discretization mesh

Table 1. Material constants used for simulation

<table>
<thead>
<tr>
<th>Material</th>
<th>Young’s modulus [GPa]</th>
<th>Thermal expansion coefficient [1/K]</th>
<th>Poisson’s ratio [-]</th>
<th>Density [kg/m³]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>380</td>
<td>6.5 × 10⁻⁶</td>
<td>0.23</td>
<td>4700</td>
</tr>
<tr>
<td>2</td>
<td>440</td>
<td>9.4 × 10⁻⁶</td>
<td>0.26</td>
<td>5200</td>
</tr>
<tr>
<td>3</td>
<td>250</td>
<td>6.2 × 10⁻⁶</td>
<td>0.21</td>
<td>7150</td>
</tr>
<tr>
<td>4</td>
<td>210</td>
<td>1.2 × 10⁻⁶</td>
<td>0.30</td>
<td>7860</td>
</tr>
</tbody>
</table>

Material’s parameters change, in transition layer between TiAlN and TiN, was modelled using sigmoidal transition function \( E(x) \). Function \( E(x) \) is a model of continuous and symmetric material parameters change. Overt formula of transition function, for Young’s modulus modification values is given by equation:

\[
E(x) = E_i + \left( E_f - E_i \right) \frac{1}{1 + \exp\left(-10^\beta x\right)} \tag{6}
\]

The \( E(x) \) function plot is shown in Figure 2 for Young’s modulus along X axis, however along Y axis materials parameters values for fixed X coordinates remain fixed. Analogously, change of the other modelled material’s parameters, like: Poisson’s ratio, thermal expansion coefficient and coating layers’ density, were assumed.

2. Multi objective optimization procedure

The goal of multi objective optimization is to calculate the optimal thickness values of TiAlN and TiN layers, which would satisfy three decisional objectives, assuming that the set of acceptable decisional variables is given as follows:

\[
D = d_1 \times d_2 = [0.2–3] \mu m \times [0.2–3] \mu m \tag{7}
\]

The first decisional objective \( K_1 \) is an average value of Huber -Von Mises stress deviation, along Y1 comparative straight line, from fixed reference stress value inside the substrate. Decisional objective \( K_1 \) is represented by the equation:

\[
K_1 = \frac{1}{n} \sum_{i=1}^{n} |\sigma_{x_i} - \sigma_{y_i}| \tag{8}
\]

where:
- \( n \) - number of node points on Y1 straight line,
- \( \sigma_{x_i} \) - Huber Von Mises stress value along Y1 comparative straight line,
- \( \sigma_{y_i} \) - stress reference value inside the substrate.

For the fixed set of decisional solutions \( D \) - given in formula (7), variation of \( K_1 \) objective value versus \( d_1 \) and \( d_2 \) decisional variables is shown in Figure 3.
negative magnitude, hence minimal stress value - means maximal absolute compression stresses value. Decisional objective $K_2$ is represented by the equation:

$$K_2 = \min \sigma_{ij} \mid x=d_i$$  \hspace{1cm} (9)

For the fixed set of decisional solutions D - given in formula (7), variation of $K_2$ objective value versus $d_1$ and $d_2$ decisional variables is shown in Figure 4.

![Figure 4. Objective $K_2$ as a function of $d_1$ and $d_2$ variables](image)

The third decisional objective $K_3$ is the minimal stress value $\sigma_{nn}$ along X2 comparative straight line. Decisional objective $K_3$ is represented by the equation:

$$K_3 = \min \sigma_{nn} \mid x=d_i$$  \hspace{1cm} (10)

For the fixed set of decisional solutions D - given in formula (7), variation of $K_3$ objective value versus $d_1$ and $d_2$ decisional variables is shown in Figure 5.

To make task solution easier, all decisional objectives were normalized in the following way:

$$K_i^{(\alpha)} = \frac{K_i - K_i^{\min}}{K_i^{\max} - K_i^{\min}}; \quad i=1, 2, 3; \quad K_i^{(\alpha)} \in [0,1]$$  \hspace{1cm} (11)

where:

$K_i^{\min}$ and $K_i^{\max}$ denote the minimum and maximum objective values for the analysed set of decisional variables D respectively.

The task of multi objective optimization is to determine set of solutions in D area, with simultaneous minimization of all decisional objectives values (equation 12):

$$K_1^{(\alpha)} \rightarrow \min, \quad K_2^{(\alpha)} \rightarrow \min, \quad K_3^{(\alpha)} \rightarrow \min$$  \hspace{1cm} (12)

Further in the paper only the normalized decisional objectives will be used, without the superscript (n) in notation. In the next step a domination relation was introduced, between any two decisional variables vectors $[15] d=[d_1, d_2]$ and $d'=[d_1', d_2']$ which belong to D set in a form:

$$d > d' \Leftrightarrow d - d' \in C \quad C = \{(a_1, a_2) \in \mathbb{R}^2 : a_1, a_2 \geq 0\}$$  \hspace{1cm} (13)

Let $K=\left[K_1, K_2, K_3\right]$ be any vector in decisional objective space, then solution $d^*$ is named minimal in Pareto sense if for every acceptable solution, the following implication is correct:

$$K(d^*) \succ K(d) \Ra K(d') = K(d)$$  \hspace{1cm} (14)

Set of all possible, optimal solutions (in Pareto sense) is also named the non-dominated solutions set (Pareto optimal). Set of dominated and non-dominated solutions, for the multi objective optimization problem in consideration, is shown in Figure 6.

To analyse the set of non-dominated solutions, Euclidean’s metric was introduced into normalized decisional objectives space with formula:

$$d(K_{0}, K) = \sqrt{\left(K_1^{(\alpha)}\right)^2 + \left(K_2^{(\alpha)}\right)^2 + \left(K_3^{(\alpha)}\right)^2}$$  \hspace{1cm} (15)

where:

$K_0$ is a point with coordinates $K_0=(0,0,0)$.

The obtained functional dependence of distance values between the points from the objective space $K=\left(K_1, K_2, K_3\right)$ and the origin of coordinate system $K_0=(0,0,0)$ is shown in Figure 7. Four examples of solution sets of $d_1$ and $d_2$ with values of tested objectives are shown in Table 2.

Table 2. Examples of Pareto-optimal solution sets

<table>
<thead>
<tr>
<th>Solution</th>
<th>$K_1$</th>
<th>$K_2$</th>
<th>$K_3$</th>
<th>$d_1$ [µm]</th>
<th>$d_2$ [µm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a)</td>
<td>0.0000</td>
<td>0.7000</td>
<td>0.2429</td>
<td>0.2000</td>
<td>3.0000</td>
</tr>
<tr>
<td>(b)</td>
<td>0.9373</td>
<td>0.0000</td>
<td>0.0050</td>
<td>2.9125</td>
<td>0.4625</td>
</tr>
<tr>
<td>(c)</td>
<td>1.0000</td>
<td>0.5093</td>
<td>0.0000</td>
<td>2.9125</td>
<td>0.2000</td>
</tr>
<tr>
<td>(d)</td>
<td>0.3943</td>
<td>0.3532</td>
<td>0.2418</td>
<td>0.2000</td>
<td>0.9000</td>
</tr>
</tbody>
</table>
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![Fig. 6. Dominated and Pareto-optimal solution sets](image1)

![Fig. 7. Functional dependence of distance values between the points from the objective space \( K = (K_1, K_2, K_3) \) and the coordinate system origin \( K_0 = (0, 0, 0) \)](image2)

Solution set (a) is assuring minimal objective \( K_1 \) value, obtained while solution sets (b) and (c) satisfy the assumption related to minimization of \( K_2 \) and \( K_1 \) objectives. The most universal is solution set (d) guaranteeing minimization of formula (15) (that point is marked in Figure 7). This solution set, is a compromise between objectives minimization, and minimization of differences between objectives values.

For solution sets from Table 2 (in Figure 8) functional relationships are presented of Huber von Mises stress values versus spatial x variable, along the Y1 comparative straight line. Finally the functional relationships of \( K_1, K_2 \) and \( K_3 \) objectives values, from decisional variables (which are Pareto-optimal solutions) are illustrated in Figures 9-11.

### 3. Conclusions

In this article, the multi objective optimization procedure, which helps in multilayer coatings architecture design process, based on thermal strains and thermal stresses states in the individual layers of the coating, was described. The task of that multi objective optimization, was to determine the optimal TiAlN and TiN layer thickness values, in respect to the assumed decisional objectives. The obtained Pareto - optimal set of solutions is presented in Figure 6. The optimal solution sets analysis, is a highly complicated and ambiguous task. To analyse this set, using the Euclidean’s metric was proposed in the space of the normalised, non-dimensional decisional objectives. Obtained
functional dependence: of distance values between the points from the objectives space $K=(K_1, K_2, K_3)$, and the origin of coordinate system $K_0=(0, 0, 0)$, is shown in Figure 7. The point from $K=(K_1, K_2, K_3)$ space, for which the distance given by the (15) formula is minimal - corresponds to (d) decisional variables set from Table 2. One can assume that (d) type solution is the best solution, chosen from all optimal solutions - regarding proposed procedure of solutions sets analysis, which depends on distance given by formula (15) minimization. The number of methods for the optimal solutions sets analysis is infinite. For different solution choice procedures we will surely obtain different results from the obtained optimal solutions sets and each of them will be correct, because the one universal selection procedure does not exist. Therefore, development of a certain selection function class as a template should be considered, which would comparison make possible of the obtained optimum solution acquired in different optimization procedures.

Fig. 8. Huber von Mises stress values versus x variable, along Y1 comparative straight line

Fig. 9. Functional dependence of objective $K_1$ value, from decisional variables (Pareto-optimal solutions)

Fig. 10. Functional dependence of objective $K_2$ values, from decisional variables (Pareto-optimal solutions)

Fig. 11. Functional dependence of objective $K_3$ values, from decisional variables (Pareto-optimal solutions)

Acknowledgements

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References

from different optimization procedures. It is possible to acquire the obtained optimum solution as a template, which will allow for the comparison of results. Therefore, the development of a certain selection function class is correct, because the universal selection procedure does not allow for the evaluation of all optimal solutions. Each of the solution choice procedures will surely obtain different results.

For different choices of the optimal solutions sets, the analysis is infinite. For different values of the distance between the points given by formula (15), minimization of the number of methods for the solutions sets analysis, which depends on the distance value, is proposed. The point of the origin of the coordinate system, for which the distance given by the formula is minimal, corresponds to the decisional variables (Pareto-optimal solutions).

Fig. 8. Huber von Mises stress values

Fig. 9. Functional dependence of objective

<table>
<thead>
<tr>
<th>$K_1$</th>
<th>$K_2$</th>
<th>$K_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>0.6</td>
<td>0.8</td>
</tr>
</tbody>
</table>

The point of the origin of the coordinate system, for which the distance given by the formula is minimal, corresponds to the decisional variables (Pareto-optimal solutions).

Fig. 10. Functional dependence of objective

<table>
<thead>
<tr>
<th>$K_1$</th>
<th>$K_2$</th>
<th>$K_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>0.6</td>
<td>0.8</td>
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