

Ł. SZPARAGA*[‡], P. BARTOSIK**, A. GILEWICZ***, J. RATAJSKI***OPTIMIZATION OF MULTI-MODULE CrN/CrCN COATINGS****OPTIMALIZACJA WIELOMODUŁOWYCH POWŁOK CrN/CrCN**

In the paper was proposed optimization procedure supporting the prototyping of the geometry of multi-module CrN /CrCN coatings, deposited on substrates from 42CrMo4 steel, in respect of mechanical properties. Adopted decision criteria were the functions of the state of internal stress and strain in the coating and substrate, caused by external mechanical loads. Using developed optimization procedure the set of optimal solutions (Pareto-optimal solutions) of coatings geometry parameters, due to the adopted decision criteria was obtained. For the purposes of analysis of obtained Pareto-optimal solutions, their mutual distance in the space of criteria and decision variables were calculated, which allowed to group solutions in the classes. Also analyzed the number of direct neighbors of Pareto-optimal solutions for the purposes of assessing the stability of solutions.

Keywords: multi-module coatings, optimization, Pareto sets, internal stress

W pracy została zaproponowana procedura optymalizacyjna wspomagająca dobór geometrii wielomodułowych powłok CrN/CrCN, osadzonych na podłożu ze stali 42CrMo4, pod kątem właściwości mechanicznych. Przyjęte kryteria decyzyjne były funkcjami stanu naprężeń oraz odkształceń wewnętrznych w powłoce i podłożu, powstałych na skutek mechanicznych obciążeń zewnętrznych. Wykorzystując opracowaną procedurę uzyskano zbiór optymalnych wartości parametrów geometrii powłok (rozwiązania Pareto-optymalne), ze względu na przyjęte kryteria decyzyjne. Do celów analizy otrzymanych rozwiązań określono ich wzajemne odległości w przestrzeni kryteriów i zmiennych decyzyjnych, co umożliwiło pogrupowanie rozwiązań w klasy. Analizowano również liczbę bezpośrednich sąsiadów rozwiązań Pareto-optymalnych w celach oceny stabilności rozwiązań.

1. Introduction

Formation of multi-functional materials properties is one of the most modern global trends in the field of materials research [1-3]. In this area, an important role is played by PVD (Physical Vapour Deposition) technology used for production of thin coatings, which are currently being developed by many scientific and industrial centers due to the wide range of applications of these coatings in machine industry, biomedical engineering and aerospace [4-7]. The present substrate /PVD coating systems are characterized by increasingly complex structure of deposited coatings [8-11]. In particular, existing technologies allow for obtaining controlled change in physico-chemical parameters of transition layers of multilayer coatings enabling a creation of so called FGM (Functionally Graded Materials). An important factor in optimizing the properties of these coatings is the selection of type and number of layers in the coating and shaping the profile of change in the material parameters of the coating layers such as hardness and Young's modulus. Extensive research on the development of multi-layer, gradient coatings are so far mostly empirical studies, though significant progress in the development of computer optimization procedures can also be observed. They enable

the analysis of different variants of the structure of the coating due to the adopted criteria in respect to the properties of the coating. Implementation of this concept allows to replace the currently used in practice very costly trial and error methods, but it requires the solution of many complex scientific and computer problems, concerning the modelling of implicit function dependencies between the properties of the coating, and its structure [12-19].

The main damages observed during the operation of coated parts are plastic deformation of the substrate, coating delamination and cracks formed in the coating. These damages can be reduced by minimizing the internal stresses and strains in the substrate/ PVD coating system by appropriate change of the architecture and geometry of the coatings and thus improve the anti-wear properties. Hence, the design of the optimal structure of multi-layer coatings requires a detailed knowledge of the distributions of the stress and strain within a multi-layer coating caused by external mechanical loads.

In the representative work in this area [20] was proposed a geometry optimization procedure of CrN/Cr multilayer coatings deposited on steel substrate subjected to external Hertzian loads. Decision variables were the thickness of the individual layers of the coating, and optimization criteria included: the

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value of the difference in deformation of two fixed points lying near the boundary the substrate /first layer and the value of von Mises stresses in the outer surface of the coating. The aim of the optimization procedure was to determine the thickness of the individual layers, while simultaneously minimizing the value of both criteria. The results of calculation are consistent with the experimental results of the coating's optimization obtained by Kuruppu al. [21]. In turn, in [22] was optimized the geometry of multilayer TiN /TiAlN deposited on the substrate HSS (High Speed Steel) previously coated with metallic chromium. The optimization process was carried using a computer model basing on FEM (Finite Element Method) implemented in COMSOL Multiphysics 4.4 and MATLAB. As the decision variables selected TiAlN and TiN layer thickness and as the decision criteria: the value of the average absolute deviation of stress Huber-von Mises along a straight comparison line going from the outer layer towards the substrate, from a fixed reference value of stress inside the substrate, and two criteria being the normal stresses in the TiN /TiAlN and Cr/TiN boundary. The aim of the optimization was to determine the thickness of individual layers (for a given thickness of the coating, similarly as in [20]), while simultaneously minimizing the value of the three criteria.

The aim of this work is to develop these concepts to optimize wear resistant coatings using new decision criteria being also the functions of the state of internal stress and strain, on the example of multi-module CrN/CrCN coatings deposited on 42CrMo4 steel substrate. For the purposes of the analysis of sets of obtained solutions were taken into account three methods, respectively based on: Euclidean metric in the space of criteria and analysis of the number and distribution of neighbors of non-dominated solutions in space criteria and the decision variables.

2. Optimization

The object of optimization is the multi-module anti-wear CrN/CrCN coating deposited on 42CrMo4 steel substrate. Fig. 1 and Fig. 2 show schema of the object with mesh, boundary conditions and loads.

In the physical model of the coating and the substrate, the following assumptions were made:

- Cr layer, CrN and CrCN are treated as continuous and homogeneous media.
- The substrate and the coating are elastic-plastic bodies.
- Boundaries separating the individual layers from each other are planes.
- There is a perfect adhesion between the substrate and the chromium layer, and a perfect cohesion between the layers of the coating.
- Cooling the coating after PVD deposition process is carried out exclusively by radiation.
- The initial internal stresses in the coating consist of stress growth (depending on the technological parameters of the process and the type of coating), and a thermal stress resulting from the difference in thermal expansion coefficients of layers and the substrate.
- The value of the growth stress is a linear function of coating thickness.

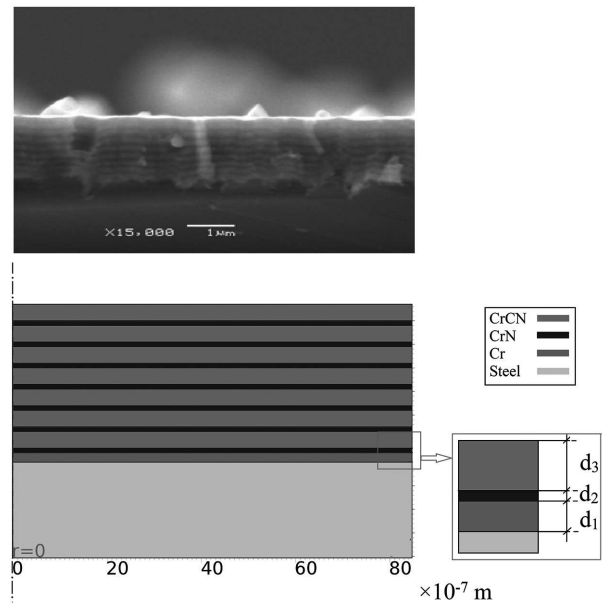


Fig. 1. Geometry of the modeled object

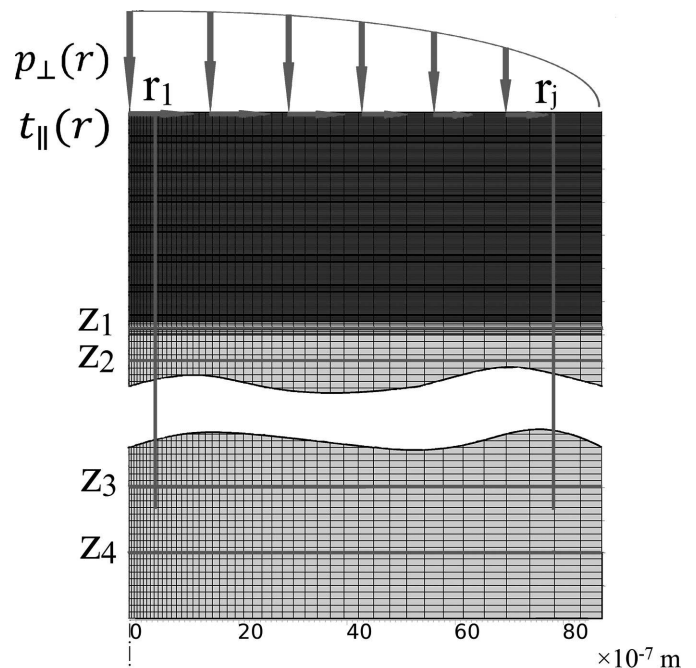


Fig. 2. Mesh of the object with comparative lines and loads

The mathematical model was developed based on the classical theory of elastic-plastic materials and FEM [23-25]. The aim of the optimization procedure was to determine the optimal thickness of the Cr, CrN and CrCN layers of and number of CrN/CrCN modules in the coating, due to the adopted decision criteria. In the considered optimization task was adopted the following set of acceptable vectors of decision variables.

$$[d_1, d_2, d_3, d_4] \in D = [0, 05; 0, 5] \mu\text{m} \times [0, 025; 0, 425] \mu\text{m} \times [0, 025; 0, 425] \mu\text{m} \times \{3, 4, 5, 6, 7\} \quad (1)$$

where d_1 (d_{Cr}) – thickness of Cr, d_2 (d_{CrN}) – thickness of CrN, d_3 (d_{CrCN}) – thickness of CrCN, d_4 – number of modules. Additionally, on d_2 and d_3 variables was imposed the

condition $d_2 + d_3 = 0.45 \mu\text{m}$, which means a constant thickness of the CrN/CrCN module. In the computer model of the object is assumed that the steel core on which the coating is deposited has a height of $100 \mu\text{m}$ and radius of $150 \mu\text{m}$. In order to formulate the mathematical form of decision criteria, a straight comparison lines (Fig. 2) were defined parallel to the radius r , with coordinates $z_1 = 100,025 \mu\text{m}$, $z_2 = 99 \mu\text{m}$, $z_3 = 90 \mu\text{m}$ i $z_4 = 80 \mu\text{m}$. In addition, was defined 20 straight comparison lines (Fig. 2) parallel to the z axis, respectively with coordinates $r_1 = 1 \mu\text{m}$, $r_2 = 3 \mu\text{m}$, etc. to $r_{20} = 40 \mu\text{m}$. Optimization was carried out at fixed constant external loads. Based on the Hertz contact theory [24] was assumed that the normal and tangential external loads acting on the coating and the substrate (Fig. 2) are of the form:

$$p_{\perp}(r) = P_0 \left[1 - \left(\frac{r}{a} \right)^2 \right]^{0.5}, \quad t_{\parallel}(r) = \mu P_0 \left[1 - \left(\frac{r}{a} \right)^2 \right]^{0.5} \quad (2)$$

where P_0 – the maximum contact pressure, μ – coefficient of friction, a – radius of contact. According to the Hertz theory, occur following relationships:

$$a = \left[\frac{3PR}{4E^*} \right]^{\frac{1}{3}}, \quad P_0 = \left[\frac{3P}{2\pi a^2} \right], \quad E^* = \left[\frac{1 - \nu_c^2}{E_c} + \frac{1 - \nu_i^2}{E_i} \right]^{-1} \quad (3)$$

where E_c and E_i respectively Young’s modulus of coating and indenter, ν_c and ν_i odpowiednio Poisson ratio for coating and indenter. The material constants of the object used in the computer model are given in Table. 1.

TABLE 1

Materials parameters

	Young’s modulus (GPa)	Thermal expansion coefficient (1/K)	Poisson’s ratio (-)	Yield strength (GPa)
Steel	210	$12 \cdot 10^{-6}$	0,3	0,415
Cr	280	$6,2 \cdot 10^{-6}$	0,23	2,3
CrN	290	$2,3 \cdot 10^{-6}$	0,22	4,5
CrCN	320	$2,6 \cdot 10^{-6}$	0,25	4,8

As the first decision criterion K_1 was adopted the average value of the maximum equivalent plastic strain ε_{eqv} on the comparative lines z_1, z_2, z_3 and z_4 (Fig. 2)

$$K_1(d_1, d_2, d_3, d_4) = \frac{\max_{z_1} \varepsilon_{eqv} + \max_{z_2} \varepsilon_{eqv} + \max_{z_3} \varepsilon_{eqv} + \max_{z_4} \varepsilon_{eqv}}{4} \quad (4)$$

This criterion concerns the assessment of development of zone of plastic deformation in the Cr adhesive layer and in the core, which indirectly is related to resistance to cracking. For example, for a 3 module coating ($d_4 = 3$) course of the value of K_1 criterion as a function of the decision variables d_1, d_2 (Fig. 3) shows a relatively strong influence of the thickness of Cr layer on the value of this criterion, which in turn does not occur for a 7 module coating ($d_4 = 7$) (Fig. 4).

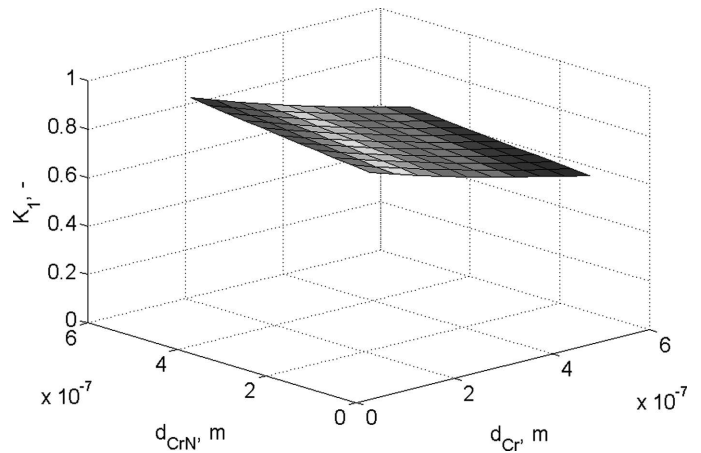


Fig. 3. Dependence of K_1 as a function of layer thickness d_1 (d_{Cr}) and d_2 , (d_{CrN}) for $d_4 = 3$ (3 module)

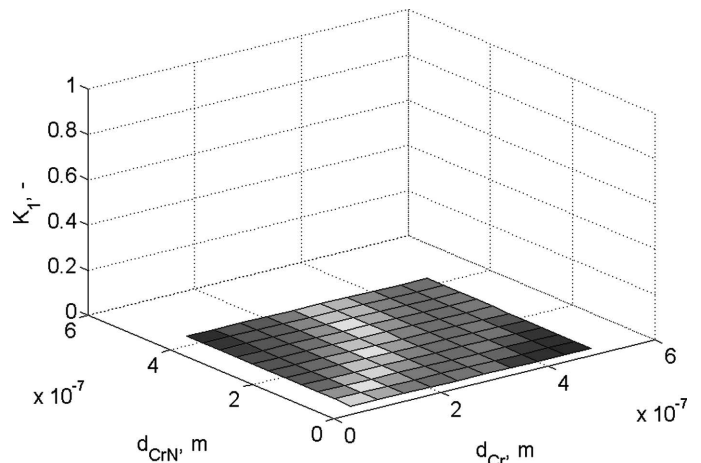


Fig. 4. Dependence of K_1 as a function of layer thickness d_1 (d_{Cr}) and d_2 , (d_{CrN}) for $d_4 = 7$ (7 module)

Based on the equivalent plastic strain distributions, it can be stated that the high value of K_1 criterion for a 3 module coating compared to the 7 module coating is caused by extensive zone of high strain in the top layers of the coating and also in the boundary between Cr adhesive layer and the core (Fig. 5). For 7 module coating zone of high plastic deformation on Cr/core boundary is much smaller, and the local maxima of these strains are several times lower (Fig. 6).

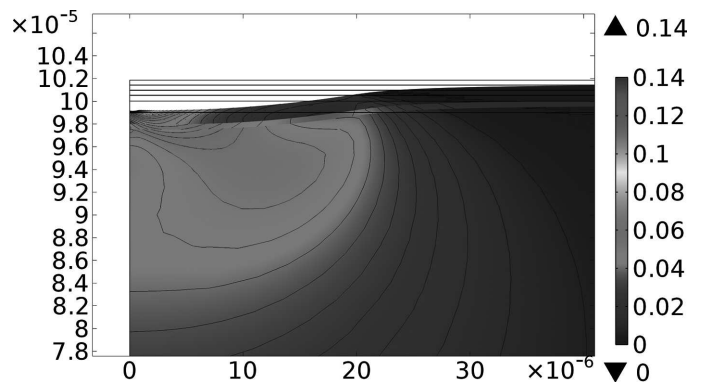


Fig. 5. Distribution of equivalent plastic strain for $d_4 = 3$ (3 module)

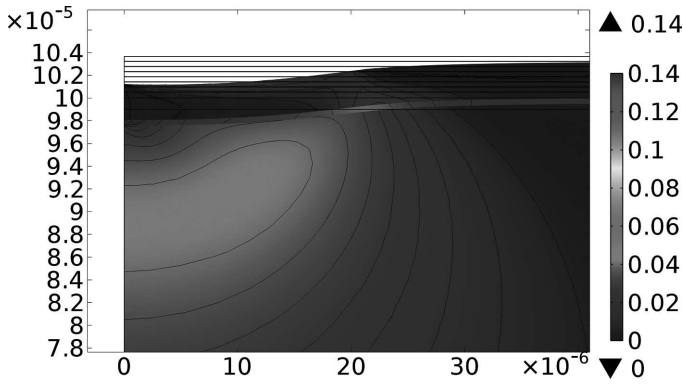


Fig. 6. Distribution of equivalent plastic strain for $d_4 = 7$ (7 module)

As the second decision criterion K_2 was adopted the maximum absolute value of the radial stress on the comparative lines r_j (Fig. 2) in the considered area of the coating.

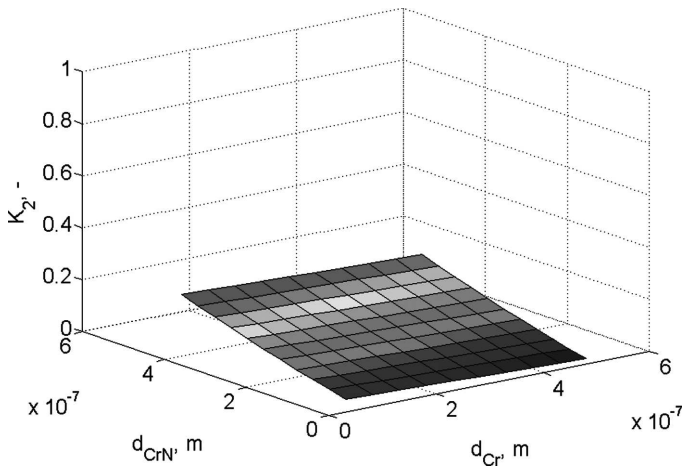


Fig. 7. Dependence of K_2 as a function of layer thickness d_1 (d_{Cr}) and d_2 , (d_{CrN}) for $d_4 = 3$ (3 module)

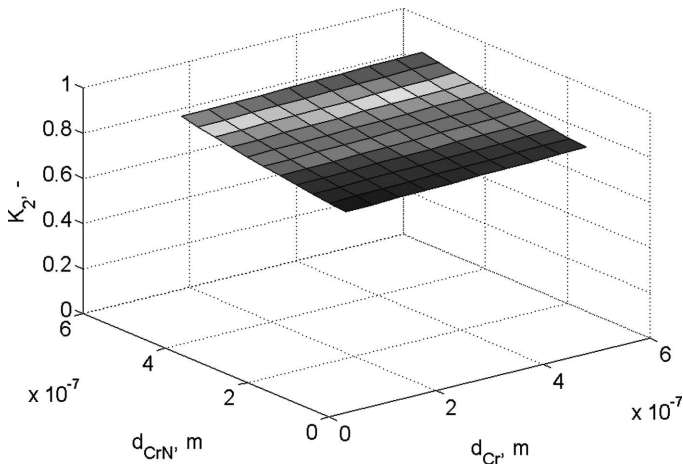


Fig. 8. Dependence of K_2 as a function of layer thickness d_1 (d_{Cr}) and d_2 , (d_{CrN}) for $d_4 = 7$ (7 module)

$$K_2(d_1, d_2, d_3, d_4) = \max_j |\sigma_r| \quad j = 1, 2, \dots, k \quad (5)$$

where j is the number of comparative line. This criterion is introduced in order to analyze the size and location of the potential formation of ring cracks caused by external mechanical

loads. For 3 module coating ($d_4 = 3$) was observed the decreasing influence of the thickness of CrN layer in the CrN/CrCr module on the value of K_2 criterion (Fig. 7) with increasing the thickness of the Cr layer. The value of the K_2 criterion for the 7 module coating ($d_4 = 7$) (Fig. 8) is several times higher in comparison to the 3 module coating ($d_4 = 3$). This is caused by the increase of compressive growth stresses with the thickness of the coating.

This effect is clearly visible in the distribution of radial stress for a 3 module coating (Fig. 9) and 7 module coating (Fig. 10).

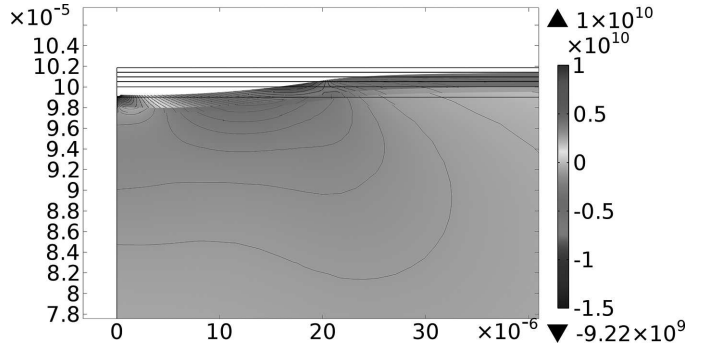


Fig. 9. Distribution of radial stress for $d_4 = 3$ (3 module)

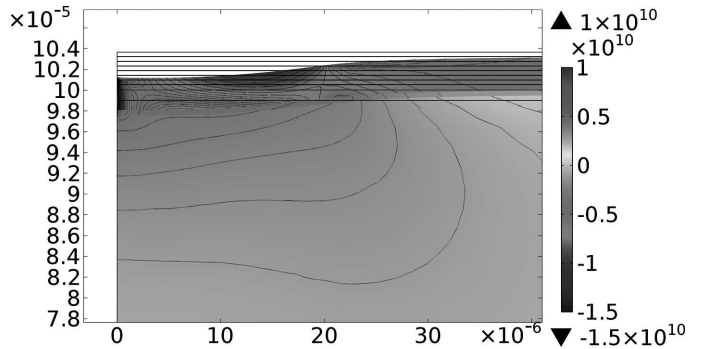


Fig. 10. Distribution of radial stress for $d_4 = 7$ (7 module)

Third decision criterion K_3 was the average, absolute value of shear stress on the comparative lines r_j (Fig. 2) in the considered area of the coating. K_3 decision criterion is given by:

$$K_3(d_1, d_2, d_3, d_4) = \frac{\sum_{j=1}^k \sum_{i=1}^N |\sigma_{rz}^{(i,j)}|}{k \cdot N} \quad j = 1, 2, \dots, k \quad i = 1, 2, \dots, N \quad (6)$$

where j is a number of the comparative line r_j , i is a number of the point from line r_j , N total number of the points from line r_j , $\sigma_{rz}^{(i,j)}$ is the value of shear stress for the i -th point from the j -th line. This criterion enables the analysis of the size and location of the potential formation of lateral cracks caused by external mechanical loads. For 3 module coating ($d_4 = 3$) the course of the value of K_3 criterion as a function of the decision variables d_1 , d_2 (Fig. 11) is approximately a plane parallel to the d_1 and d_2 , which shows a low impact of the thickness of Cr and CrN layer on the value of the criterion. For 7 module coating ($d_4 = 7$) the course of the value of K_3 criterion as a function of decision variables d_1 , d_2 (Fig. 12)

also has a shape close to a plane, however, the value of this criterion is much higher than for a coating with 3 modules ($d_4 = 3$).

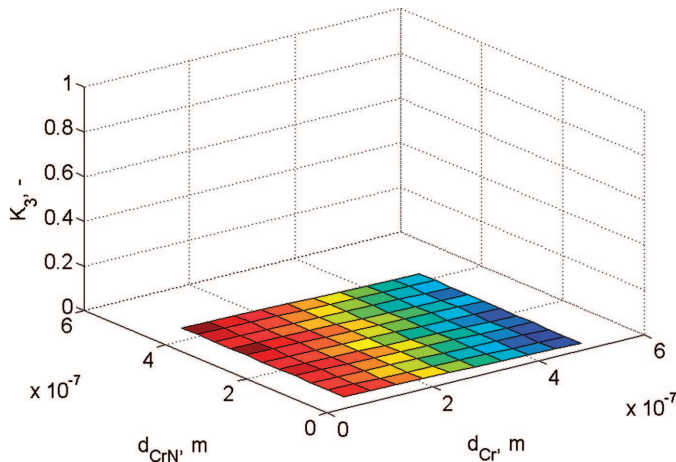


Fig. 11. Dependence of K_3 as a function of layer thickness d_1 (d_{Cr}) and d_2 , (d_{CrN}) for $d_4 = 3$ (3 module)

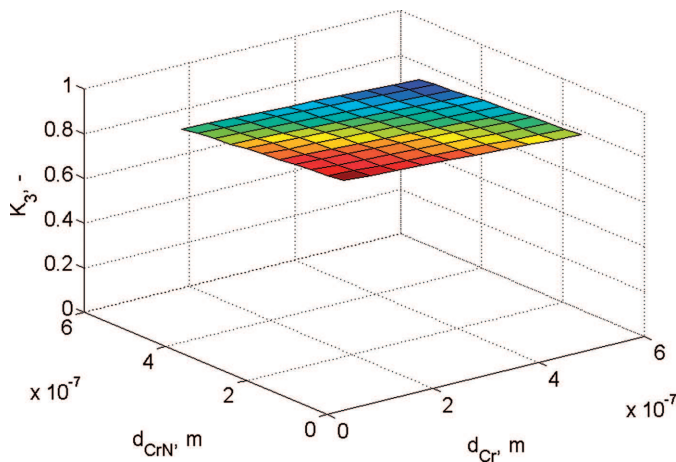


Fig. 12. Dependence of K_3 as a function of layer thickness d_1 (d_{Cr}) and d_2 , (d_{CrN}) for $d_4 = 7$ (7 module)

This is a consequence of the increase in the number of modules, because according to the assumptions the value of growth stress is greater for thicker coatings. Additionally, for a 3 module coating zone of high shear stress is located also in a large part of the core (Fig. 13), while for the 7 module coating, dominance area of high stress is present mainly in the coating (Fig. 14)

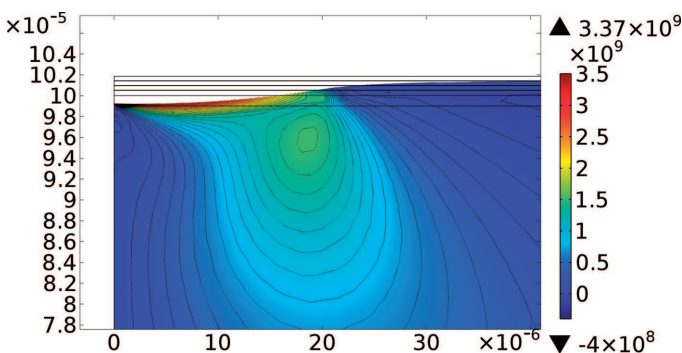


Fig. 13. Distribution of shear stress for $d_4 = 3$ (3 module)

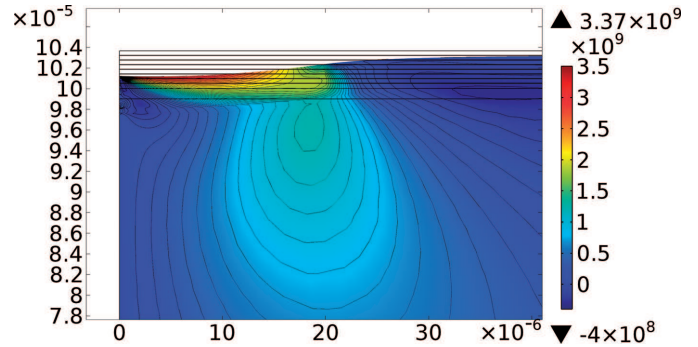


Fig. 14. Distribution of shear stress for $d_4 = 7$ (7 module)

High values of these stresses are especially disadvantageous if there are occurring on the boundaries between layers or on the boundary between Cr and the substrate, because this increases the probability of initiation and propagation of lateral cracks.

3. Results and discussion

In order to facilitate the solution of the optimization problem the decision criteria have been rescaled to the dimensionless variables and normalized as follows:

$$K_i^{(n)} = \frac{K_i - K_i^{\min}}{K_i^{\max} - K_i^{\min}} \quad i = 1, 2, 3 \quad K_i^{(n)} \in [0; 1] \quad (7)$$

In the rest of work will be used only normalized decision criteria, and hence was abandoned upper index (n) with K. The optimization problem consists in determining a set of solutions in the set D (Eq. (1)), while simultaneously minimizing the values of decision criteria, i.e.:

$$K_1 \rightarrow K_{1\min}, K_2 \rightarrow K_{2\min}, K_3 \rightarrow K_{3\min} \quad (8)$$

In general, to achieve the minima of all criteria at the same time is possible only in the case where there are no so called. conflicting criteria, in another case, each component of the vector criterion may reach its minimum at a different value of the vector of decision variables. However, there exist methods to facilitate the evaluation of acceptable (non-dominated) solutions (Pareto-optimal solutions: the solutions for which improvement of one of the criteria is inextricably linked to the deterioration of the others) for minimizing all the criteria simultaneously [20, 22, 23, 26].

As the first method of analyzing a set of non-dominated solutions (Pareto-optimal) adopted the so-called. method of "utopian solution." In the considered optimization task the "utopian solution" is located in the center of the coordinate system in the space of criteria, i.e. all three criteria are equal to zero. For this purpose, in the space of normalized decision criteria E an Euclidean metric was introduced in the form:

$$d(\vec{K}_0, \vec{K} = [K_1, K_2, K_3]) = \sqrt{K_1^2 + K_2^2 + K_3^2} \quad (9)$$

Selected types of non-dominated solutions are given in Table 2

TABLE 2
 Selected types of non-dominated solutions including boundary solutions

K_1	K_2	K_3	d_1 (d_{Cr}), μm	d_2 (d_{CrN}), μm	d_3 (d_{CrCN}), μm	d_4	type
0,3061	0,0943	0,2444	0,5	0,025	0,425	4	(a)
0,0000	0,8847	0,9434	0,5	0,025	0,425	7	(b)
0,6736	0,0000	0,0018	0,5	0,025	0,425	3	(c)
0,6797	0,0154	0,0000	0,5	0,065	0,385	3	(d)

Using the metric Eq. (9) and determining the global minimum we are looking for a solution that is closest to the utopian solution in the space of criteria. This solution is classified as type (a) (Table 2), which is a compromise between the minimization of all criteria, and minimizing the differences between their values.

Another class of non-dominated solutions are so-called "boundary solutions", ie. solutions which have at least one value of the criterion equal to zero (type (b), (c) and (d), Table 2). In an exemplary set of solutions for the solution of type (b) the minimum (zero) value takes K_1 criterion, which corresponds to a small region of high plastic deformation on the boundary between Cr layer and the core, and sets of solutions (c) and (d) satisfy respectively the minimization of K_2 and K_3 criterion (low internal stress value).

As a second alternative method of choosing the best solution from the whole set of non-dominated solutions was adopted an analysis of the number of direct neighbors of non-dominated solutions. For this purpose, for each of the non-dominated solutions (Pareto-optimal) was determined number of direct neighbors, which are also non-dominated solutions (Fig. 15). For the purposes of the analysis of to each solution has been assigned sequence number in order to facilitate graphical presentation of the results.

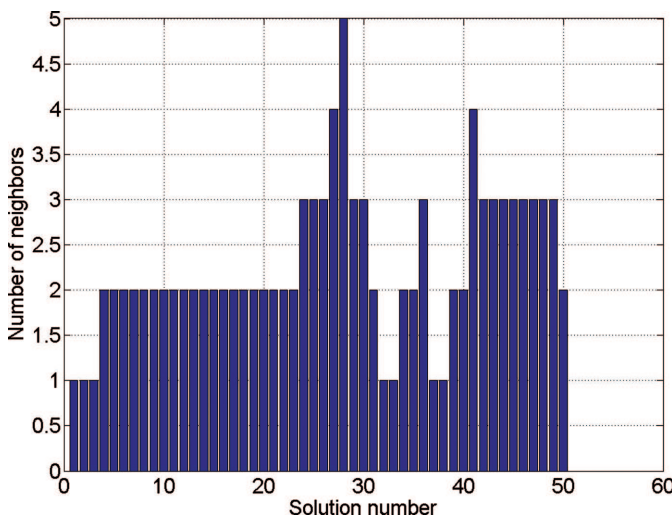


Fig. 15. Number of the direct neighbours for the Pareto optimal solutions

Examples of solution with the highest number of direct neighbors contains Table 3. It should be emphasized that non-dominated solutions possessing many neighbors are less sensitive to the potential instability of the technological pa-

rameters, because a slight change in the technological parameters with high probability would lead to a Pareto-optimal solution

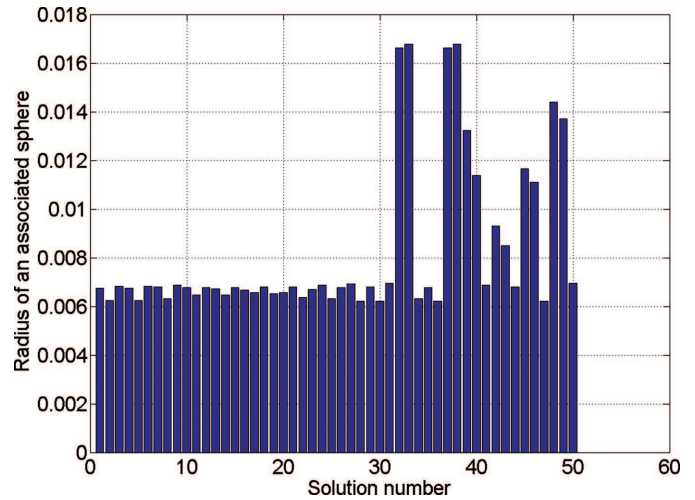


Fig. 16. Values of radius of the associated spheres for the Pareto optimal solutions

TABLE 3
 Non-dominated solutions with the highest number of direct neighbors

Number of neighbors	d_1 (d_{Cr}), μm	d_2 (d_{CrN}), μm	d_3 (d_{CrCN}), μm	d_4
5	0,45	0,065	0,385	7
4	0,45	0,025	0,425	7
4	0,5	0,025	0,425	7

The third method of analysis of a set of non-dominated solutions is based on the study of the distance from each non-dominated solution to the nearest neighbors being also non-dominated solutions. Then, with every non-dominated solution in the spaces of normalized decision criteria E_j was associated a sphere of radius equal to the minimum distance to the nearest neighbor, which is also a non-dominated solution. As before, for the graphical representation of the results each solution has been associated with sequence number. Using the proposed method of analysis for all non-dominated solutions were determined radius values of associated spheres (Fig. 16). Most of the non-dominated solution (39 of a total of 51) has a radius of the associated sphere at the level of 0.006 and 0.007 hence the volume of the associated spheres are at level $9 \cdot 10^{-7}$ and $14 \cdot 10^{-7}$, with a total volume of criterion space equal to 1. This proves the possession of neighbor characterized by almost the same values of criteria, so from the point of view of anti-wear properties these solutions may be considered as equivalent. For a more detailed analysis of obtained histogram (Fig. 16) was also generated a set of non-dominated solutions with associated spheres in the space of normalized decision criteria (Fig. 17).

The obtained non-dominated solution were group into 5 classes A-E. To class A belongs 25 solutions, B and C classes have 11 solutions and classes D and E contain 2 solutions (Fig. 17). Solutions in classes A and B are characterized by a low value of K_1 criterion, (small value of the plastic strain on the Cr/core boundary) which has been achieved by increas-

ing the number of modules (6, 7) and a high internal stress (high value of K_2 and K_3). Solutions belonging to C class occupy the central area of criteria space which corresponds to moderate values of all three criteria. In the class D is located a non-dominated solution which lies closest to the "utopian solution" (minimizing the metric (9)), while in the class E there are two boundary solutions, for one of them $K_2 = 0$ and for the another one $K_3 = 0$, which corresponds to the states with the lowest values of internal stresses.

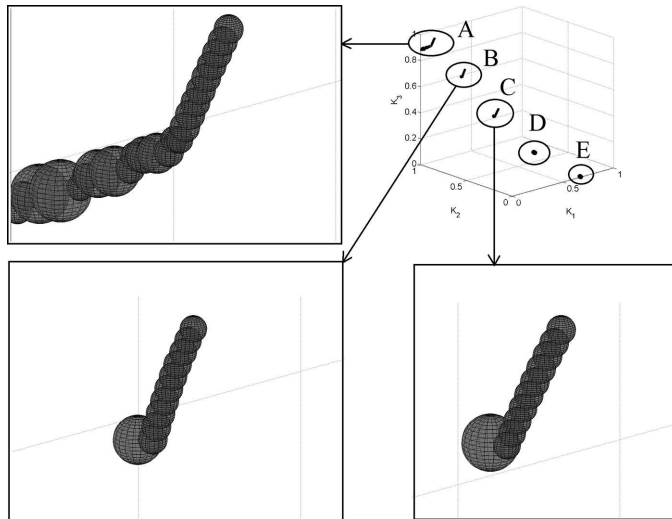


Fig. 17. Set of the associated spheres in the space of decision criteria

4. Conclusions

Using the optimization procedure developed for multi-module CrN/CrCN coating, optimal values of number of modules, thicknesses of CrN and CrCN layers forming the module, and the thickness of the Cr adhesive layer between the steel core and the coating have been specified, due to the adopted decision criteria. In order to analyze a set of non-dominated solutions (Pareto-optimal coatings) were proposed three methods to study a set of solutions. The first method was based on the study of a minimum of the Euclidean metric in the space of normalized decision criteria, thereby enabling designation of the solution being a compromise between the minimization of criteria values, and minimizing the differences between the values of the criteria. The second method of analysis was based on the analysis of the number of direct neighbors of non-dominated solutions. With this method, it was possible to nominate solutions with the highest number of neighbors, which from a practical point of view, making them the least vulnerable to the potential instability of the technological parameters of coating deposition processes. The third method of analysis of non-dominated solutions, was based on the analysis of associated spheres in the space of normalized decision criteria and enabled to group them into classes. The solutions included in the each class are characterized by similar values of criteria, which from a practical point of view means similar coatings properties. The presented optimization procedure indicates that prototyping of the geometry of the coatings is a highly ambiguous task, due to

the presence of opposing decision criteria. In this case it was the criterion K_1 (for assessing the zone of plastic deformation) and the criteria K_2 and K_3 related to the internal state of radial and shear stresses. In all such case, we obtain a set of optimal solutions (Pareto set), which consists of solution that cannot be compared to one another, because choosing the best among them is inextricably linked to the method of evaluation.

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