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Ł. Szparaga*, J. Ratajski

*Koszalin University of Technology, Institute of Technology and Education, Department of Materials and Processes Design,75-453 Koszalin, Poland, * lukasz.szparaga@tu.koszalin.pl*

PARETO OPTIMAL MULTI-OBJECTIVE OPTIMIZATION OF ANTIWEAR TiAlN/TiN/Cr COATINGS

ABSTRACT

The multi-objective optimization procedure of geometry of TiAlN/TiN/Cr multilayer coatings was created. The procedure was applied to the multilayer coatings subjected to constant tangential and normal loads (Hertzian contact). In physical model Cr, TiN and TiAlN layers were treated as a continuous medium, thus in mathematical description of the stress and strain states in the coatings a classical theory of stiffness was used. Decisional variables used in procedure were thicknesses of Cr, TiN and TiAlN layers and decisional criteria were functions of the stress and strain fields in the coating and substrate. Using created optimization procedure, Pareto set of optimal values of layers' thicknesses were determined. Additionally, two methods of analysis of Pareto-optimal set were introduced and discussed.

Key words: *multi-objective optimization, multilayer coatings, internal stress, Pareto sets*

INTRODUCTION

Nowadays, surface engineering is one of the most dynamically developing area of science and industry. Of particular interest are protective coatings deposited via PVD techniques, because of their wide range of applications [1,2]. However, despite the rapid development of coating deposition techniques, there is still a number of unresolved problems with intelligent designing of architecture and geometry of multilayer and gradient coatings. Among them, the key problem is the physical and mathematical description of the mechanisms of internal stress and strain evolution in the coatings during the deposition process, as well as determining the state of stress due to different thermal and mechanical loads. [3-9]. Despite the significant development of computational techniques (artificial intelligence, cellular automata, finite element method) there is a continuing need for the creation of more excellent mathematical and computer models designed for the optimization procedures. For this reason, there is relatively little papers on computer poly-optimization of wear resistant coatings on the basis of mathematical models describing the stress and strain states due to external loads [10-15]. Deliberate therefore becomes to develop new or modify existing procedures for multi-objective optimization (poly-optimization) supporting designing of multilayer coatings, including the development of new methods of analysis of received sets of solutions.

MULTI-OBJECTIVE OPTIMIZATION

The objects of multi-objective optimization are antiwear TiAlN/TiN/Cr coatings. A detailed physical and mathematical model of the analyzed objects is presented in [4,9,13-15]. Fig.1 shows a diagram of the object with the applied mesh, boundary conditions and loads.

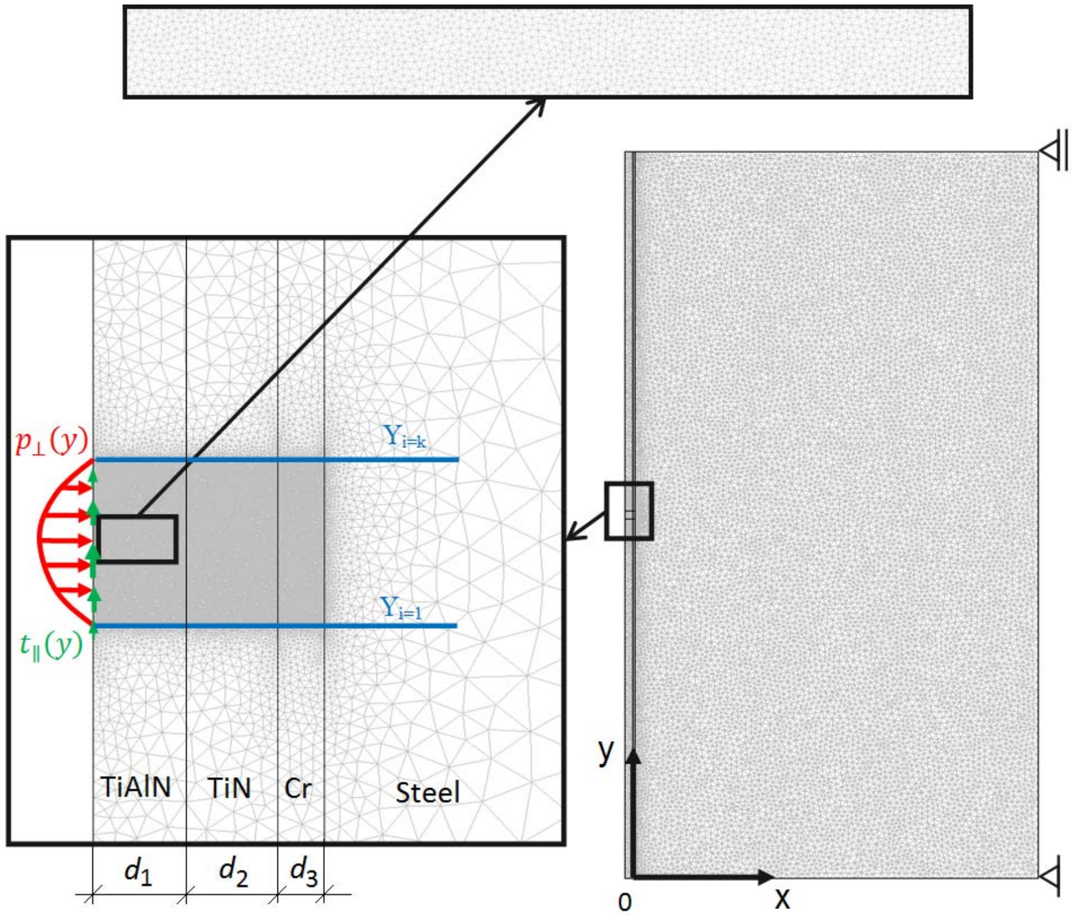

Fig. 1. Scheme of the modelled object

The aim of the multi-objective procedure was to determine the optimal thickness of the TiAlN, TiN, and Cr layers in the TiAlN/TiN/Cr coating due to the postulated decision criteria. In the considered poly-optimization task the following set of acceptable vectors of decision variables was assumed:

$$[d_1, d_2, d_3] \in D = [0{,}2;\, 1{,}0]\mu m \times [0{,}2;\, 1{,}0]\mu m \times [0{,}2;\, 1{,}0]\mu m \tag{1}$$

where: d_1 - TiAlN layer thickness, d_2 - TiN layer thickness, d_3 - Cr layer thickness. Multi-objective optimization of the coatings was carried out at fixed constant external loads. Based on Hertz contact theory [9,10], it was assumed that the normal and tangential external loads acting on the coating and the substrate have a following form:

$$p_\perp(y) = P_0\left[1-\left(\frac{y}{a}\right)^2\right]^{0,5},\ t_{//}(y) = \mu P_0\left[1-\left(\frac{y}{a}\right)^2\right]^{0,5} \tag{2}$$

where: P_0 - maximum contact pressure, μ - friction coefficient, a - radius of the intender penetration. According to the Hertzian contact theory the following notation was adopted:

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

where: E_c ,ν_c and E_i ,ν_i are respectively Young's modulus and Poisson's ratio of the coating and indenter. Based on the proposed set of decision criteria from [15], the first decision criterion K_1 was the maximum value of von Mises stress gradient in the analyzed area of the coating:

$$K_1(d_1,d_2,d_3)=\max_{i,j}\frac{\left|\sigma_{vm(j)}^{(i+3)}-\sigma_{vm(j)}^{(i)}\right|}{x_{(j)}^{(i+3)}-x_{(j)}^{(i)}} \quad j=1,2,\ldots,k \tag{4}$$

where: i is the number of point calculated from the coating surface along a straight comparative line Y_j, j is the number of comparative line, $\sigma^{(i)}{}_{vm(j)}$ is the value of von Mises stress for the i-th point from comparative line of the number j, $x^{(i)}{}_{(j)}$ is the value of x coordinate for the i-th point lying on the j-th straight comparative line. Fig. 2 shows, for a fixed set of decision variables D, dependence of K_1 criterion value as a function of decision variables d_1, d_2, d_3, for subsets $\{d_1, d_2, d_3 = d_{3\min}\}$ and $\{d_1, d_2, d_3 = d_{3\max}\}$.

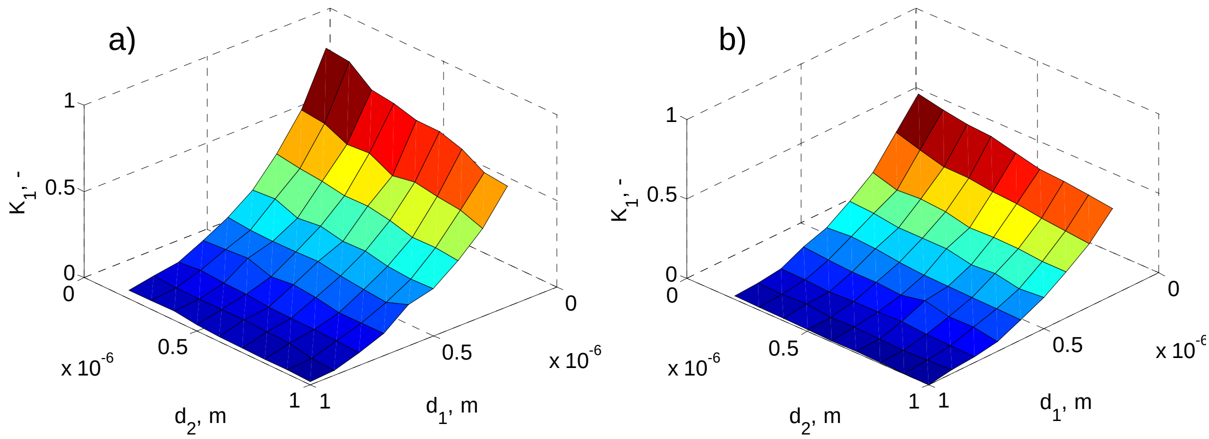

Fig. 2. Dependence of K_1 as a function of layer thickness d_1 and d_2, for a) $d_3=d_{3min}$, b) $d_3=d_{3max}$

The second decision criterion K_2 was the maximum value of the difference of linear deformation along the x-axis for points P_{1j} and P_{2j} lying on comparative line Y_j in the analyzed area of the coating:

$$K_2(d_1,d_2,d_3)=\max_j\left|\varepsilon_{x1(j)}-\varepsilon_{x2(j)}\right| \quad j=1,2,\ldots,k \tag{5}$$

where: j is the number of comparative line, $\varepsilon_{x1(j)}$ is linear deformation along the x-axis in point $P_{1j}=(d_1+d_2+d_3-75nm,Y_j)$ and $\varepsilon_{x2(j)}$ is linear deformation along the x-axis in point $P_{2j}=(d_1+d_2+d_3+200nm,Y_j)$. Fig. 3 shows, for a fixed set of decision variables D, dependence of K_2 criterion value as a function of decision variables d_1, d_2, d_3, for subsets $\{d_1, d_2, d_3 = d_{3\min}\}$ and $\{d_1, d_2, d_3 = d_{3\max}\}$. It should be marked that for better visualization of the K_2 dependence in fig. 3 (b) axes are inverted with respect to the axes in fig.3 (a).

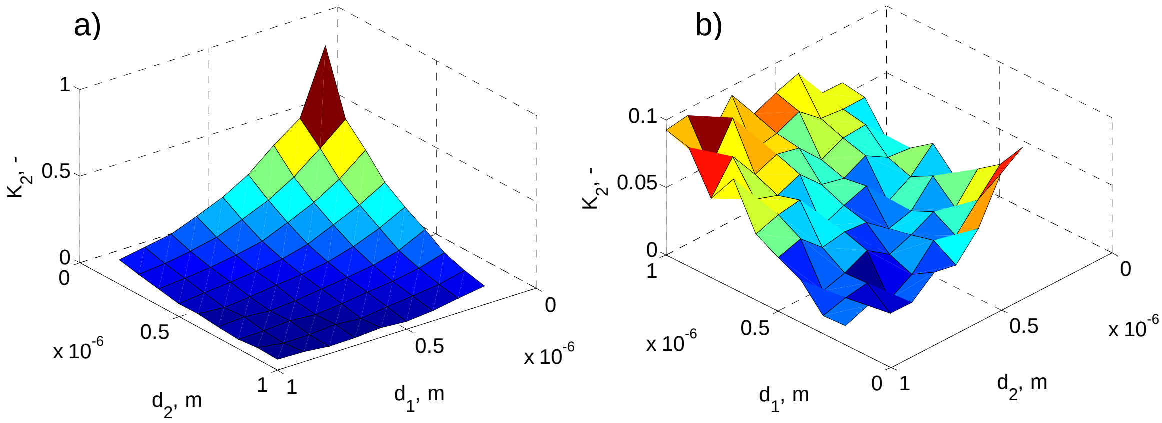

Fig. 3. Dependence of K_2 as a function of layer thickness d_1 and d_2, for a) $d_3=d_{3min}$, b) $d_3=d_{3max}$

The third decision criterion K_3 was the maximum value of mean squared deviation of normal stress σ_y for points lying on the straight comparative line Y_j, from fixed reference value of stress inside the substrate. K_3 decision criterion is given by:

$$K_3(d_1, d_2, d_3) = \max_j \frac{1}{n_r}\left(\sum_{i=1}^{n_r}\sigma_{y(j)}^{(i)} - \sigma_{y(j)}^{(n_r)}\right)^2 \quad j = 1,2,\ldots,k \tag{6}$$

where: i is the number of point counted from the coating surface along a straight comparative line Y_j, j is the number of comparative line, $\sigma^{(i)}_{y(j)}$ is the value of normal stress along the y-axis for the i-th point, lying on a comparative line Y_j, $\sigma^{(n_r)}_{y(j)}$ is the value of normal stress along the y-axis for the n_r-th point, lying on a comparative line Y_j, whose coordinates are $P_{nr}=(d_1+d_2+d_3+200nm, Y_j)$. Fig. 4 shows, for a fixed set of decision variables D, dependence of K_3 criterion value as a function of decision variables d_1, d_2, d_3, for subsets $\{d_1, d_2, d_3 = d_{3min}\}$ and $\{d_1, d_2, d_3 = d_{3max}\}$.

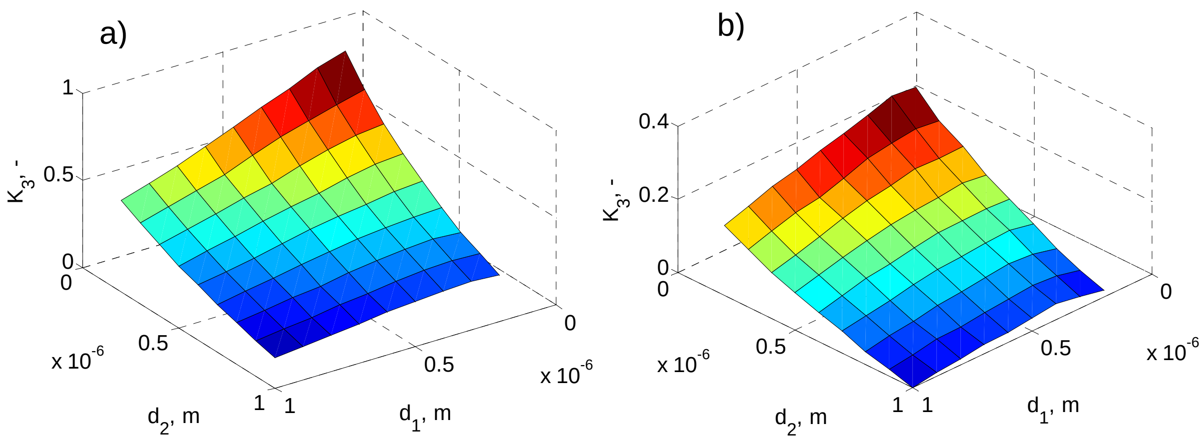

Fig. 4. Dependence of K_3 as a function of layer thickness d_1 and d_2, for a) $d_3=d_{3min}$, b) $d_3=d_{3max}$

To facilitate the solution of the multi-objective optimization problem the decision criteria were rescaled to dimensionless variables and normalized as follows:

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

In order to unify notation, from now on will be used only normalized decision criteria, thus abandoned was the upper index (n) of the *K*. Multi-objective optimization task was to determine the set of solutions in *D* for simultaneous minimization of all decision criteria, i.e.:

$$K_1 \to K_{1\min}\ , K_2 \to K_{2\min}\ , K_3 \to K_{3\min} \tag{8}$$

In general, this problem is usually very difficult or impossible to solve, because each component of the vector criteria can achieve its minimum at a different value of the vector of decision variables. However, there are several methods that facilitate the assessment of acceptable solutions for minimizing all criteria at the same time [10,13,14]. Among them, particularly noteworthy is a method of solving multi-criteria problems based on so-called Pareto sets [13,14].

RESULTS

For the considered multi-objective optimization task the set of all of acceptable solutions is presented in fig. 5.

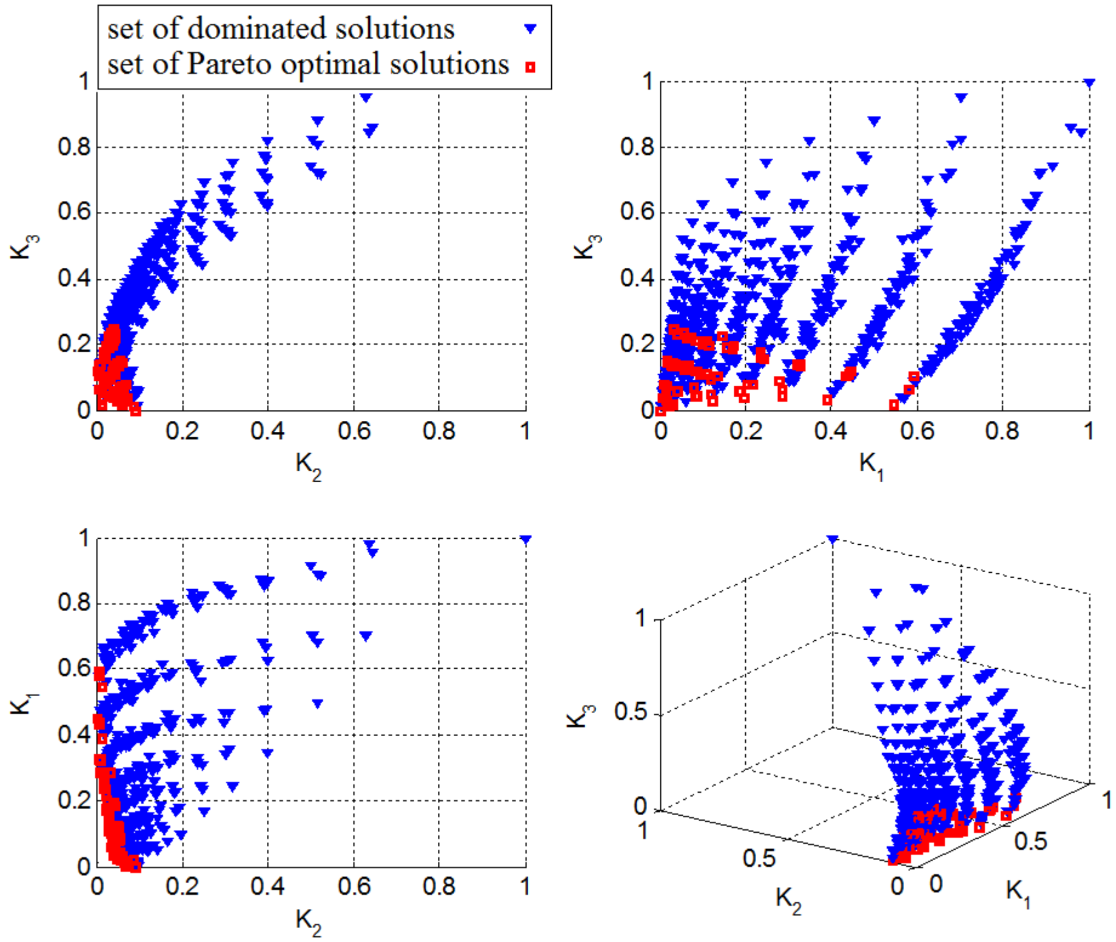

Fig. 5. Set of acceptable solutions

In order to analyze the set of Pareto-optimal (nondominated) solutions in the space of normalized decision criteria K an Euclidean metric was introduced in the following form:

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

The selected types of Pareto-optimal solutions contains tab.1.

Table 1. *Examples of specific Pareto optimal solutions*

K_1	K_2	K_3	d_1, μm	d_2, μm	d_3, μm	type
0,0311	0,0584	0,0187	0,8	1,0	1,0	a
0,0000	0,0926	0,0000	1,0	1,0	1,0	b
0,4467	0,0000	0,1192	0,3	0,7	1,0	c

The most universal Pareto-optimal solution is type (a), ensuring minimization of the metric (9). This solution is a compromise between minimizing the criteria values and minimization of differences between them. Whereas solutions (b) and (c) provide a minimum value respectively by the criteria K_1, K_2 and K_3. It is worth noting that the method of solutions analysis using the metric (9) allows usually identify a single solution, for which the metric's value is minimal, which is extremely useful in the analysis of highly complex sets of solutions. The second method of analysis of Pareto-optimal solutions set (nondominated solutions) is based on an examination of distance from each Pareto-optimal solution to the neighbors that are Pareto-optimal solutions. For the purpose of graphical representation of the results each Pareto-optimal solution was assigned with a number. Subsequently with each nondominated solution from the space of normalized decision criteria K a ball was associated which radius was equal to the minimum distance to the nearest neighbor which is also a nondominated solution (fig.6).

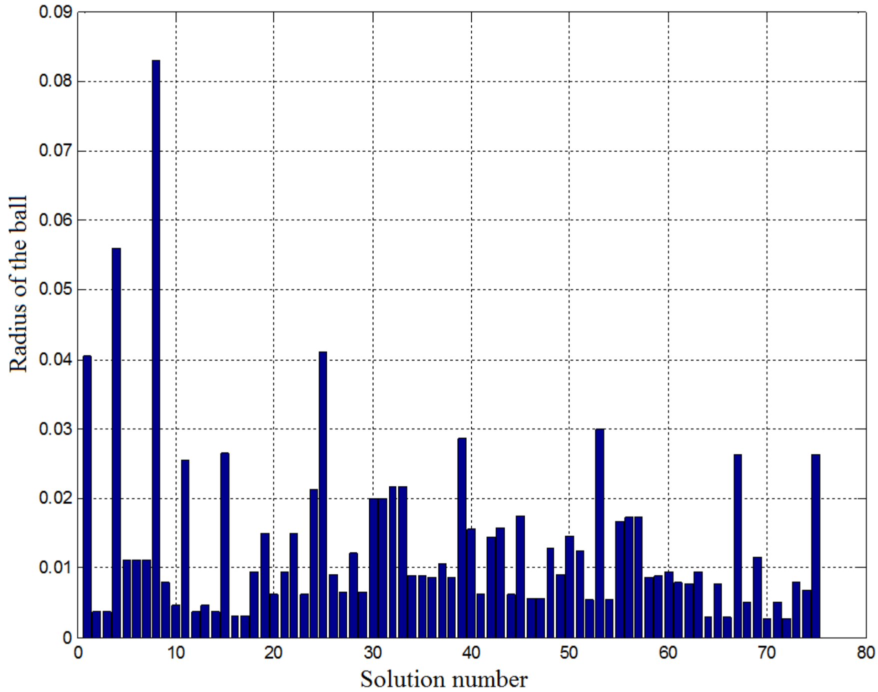

Fig. 6. Value of radius of the associated ball for the Pareto optimal solutions

In order to analyze the histogram (fig.6) a set of nondominated solutions with associated balls in the spaces of normalized decision criteria (fig.7) was also generated. This method is an effective method of selection the nondominated solutions which have in their close proximity at least one solution which is nondominated.

CONCLUSIONS

Using created multi-objective optimization procedure an optimal thicknesses of the Cr, TiN and TiAlN layers of due to the adopted decision criteria were specified. In order to analyze the set of nondominated solutions (Pareto-optimal solutions) two methods of analysis of solutions were proposed. The first method was based on an examination of a minimum of Euclidean metric in the space of normalized decision criteria, thereby enabling determination of the solution being a compromise between minimization of the criteria values and differences between them. In addition, it should also be emphasized that the solution of this type can be characterized by high instability with little change of technological parameters of the process.

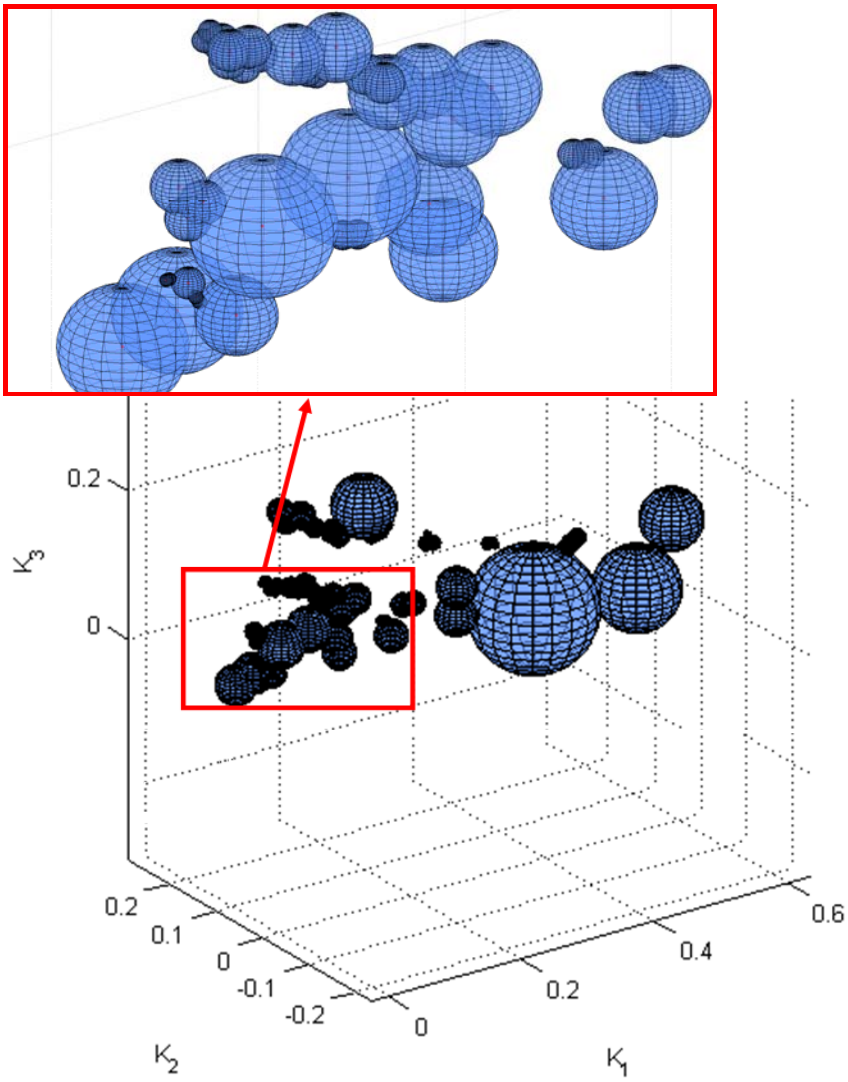

Fig. 7. Set of the associated balls in the space of decisional criteria

The second method of analysis was based on distance analysis between the Pareto-optimal solutions in the space of normalized decision criteria. It enables the analysis of the geometry of the set of Pareto-optimal solutions, which is crucial from the point of view of the stability of the solution. It should also be stressed that the proposed methods are only a starting point for further research on the analysis of sets Pareto-optimal solutions, which is necessary due to the potential applications in programs for intelligent coatings design.

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REFERENCES

1. Dobrzańska-Danikiewicz A.D.: The development perspectives of Physical Vapour Deposition technologies. Journal of Achievements in Materials and Manufacturing Engineering 54 (2012), 103-109.
2. Bell T., Mao K., Sun Y.: Surface engineering design: modelling surface engineering systems for improved tribological performance. Surface & Coatings Technology 108-109 (1998), 360-368.
3. Bennani H. H. Takadoum J.: Finite element model of elastic stresses in thin coatings submitted to applied forces. Surface and Coatings Technology 111 (1999), 80-85.
4. Djabella H., Arnell R. D.: Finite element analysis of the contact stresses in elastic coating/substrate under normal and tangential loads. Thin Solid Films 223 (1993), 87-97.
5. Komvopoulos K.: Elastic-plastic finite element analysis of indented layered media. Journal of Tribology, 111 (1989), 430-440.
6. Śliwa A., Dobrzański L.A., Kwaśny W., Staszuk M., Simulation of the microhardness and internal stresses measurement of PVD coatings by use of FEM, Journal of Achievements in Materials and Manufacturing Engineering 43 (2) (2010), 684-691.
7. Śliwa, A., Dobrzański, L. A., Kwaśny, W., Sitek, W.: The computer simulation of internal stresses on the PVD coatings. Archives of Computational Materials Science and Surface Engineering, 1(3) (2009), 183-188.
8. Dobrzański, L. A., Śliwa, A., Sitek, W.: Finite Element Method application for modeling of PVD coatings properties. Proceedings of the 5th International Surface Engineering Conference (2006), 26-29.
9. Johnson K. L.: Contact Mechanics, Cambridge, 1985.
10. Lakkaraju R. K., Bobaru F., Rohde S. L.: Optimization of multilayer wear-resistant thin films using finite element analysis on stiff and compliant substrates. Journal of Vacuum Science & Technology A: Vacuum, Surfaces, and Films 24 (2006), 146-155.
11. Kuruppu M. L., Negrea G., Ivanov I. P., Rohde S. L.: Monolithic and multilayer Cr/CrN, Cr/Cr_2N, and Cr_2N/CrN coatings on hard and soft substrates. Journal of Vacuum Science and Technology A 16 (1998), 1949-1956.
12. Valle R., Leveque D., Parlier M.: Optimizing substrate and intermediate layers geometry to reduce internal thermal stresses and prevent surface crack formation in 2-D multilayered ceramic coatings. Journal of the European Ceramic Society 28 (2008), 711-716.

13. Szparaga Ł., Ratajski J., Zarychta A.: Multi objective optimization of, wear resistant TiAlN and TiN coatings deposited by PVD techniques. Archives of Materials Science and Engineering 1/48 (2011), 33-39.
14. Szparaga Ł., Ratajski J.: Polyoptimization of antiwear TiAlN and TiN coatings, deposited by PVD techniques on tools for wood machining. Measurement Automation and Monitoring (Pomiary Automatyka Kontrola) 57 (2011) (in Polish), 1055-1058.
15. Szparaga Ł., Ratajski J.: Polyoptimization of gradient antiwear TiAlN/TiN coatings. Materials Science (Inżynieria Materiałowa) 5/195 (2013), (in Polish).