Archives of Materials Science and Engineering

Volume 48
Issue 1
March 2011
Pages 33-39

International Scientific Journal published monthly by the World Academy of Materials and Manufacturing Engineering

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

Ł. Szparaga [a,*], J. Ratajski [a], A. Zarychta [b]

[a] Institute of Mechatronics, Nanotechnology and Vacuum Technique, Koszalin University of Technology, ul. Racławicka 15-17, 75-620 Koszalin, Poland

[b] Institute of Engineering Materials and Biomaterials, Silesian University of Technology, ul. Konarskiego 18a, 44-100 Gliwice, Poland

* Corresponding author: E-mail address: lukasz.szparaga@tu.koszalin.pl

Received 06.12.2010; published in revised form 01.03.2011

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:

Ł. Szparaga, J. Ratajski, A. Zarychta, Multi objective optimization of wear resistant TiAlN and TiN coatings deposite by PVD techniques, Archives of Materials Science and Engineering 48/1 (2011) 33-39.

METHODOLOGY OF RESEARCH, ANALYSIS AND MODELLING

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:

$$\sigma = \left[\sigma_x \sigma_y \sigma_z \sigma_{xy} \sigma_{yz} \sigma_{xz}\right]^T \tag{1}$$

where:

σ_x, σ_y, σ_z - normal stress along x,y,z axes, respectively,
σ_{xy}, σ_{yz}, σ_{xz} - shear stress along xy,yz,xz planes, respectively.

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

$$\varepsilon = \left[\varepsilon_x \varepsilon_y \varepsilon_z \varepsilon_{xy} \varepsilon_{yz} \varepsilon_{xz}\right]^T \tag{2}$$

where:

ε_x, ε_y, ε_z - normal strain (strain of edges of the analysed element), along x,y,z axes, respectively,
ε_{xy}, ε_{yz}, ε_{xz} - shear strain, describing angle change, between walls of analysed element.

Thermal strain is defined by the vector:

$$\varepsilon^{th} = \Delta T\left[\alpha_x \alpha_y \alpha_z\, 0\, 0\, 0\right]^T \tag{3}$$

where:

α_x, α_y, α_z - thermal expansion coefficients, along x, y, z axes, respectively,
$\Delta T = T - T_{ref}$ - temperature increment,
T_{ref} - reference temperature.

Generalized Hook's law is given by a formula:

$$\sigma = D\varepsilon^{th} \tag{4}$$

where:

D - stiffness matrix containing: Young's and Kirchhoff's modulus and Poisson's ratios [11-14].

Knowing the form of σ vector, Huber Von Mises stresses values, can be calculated with the formula:

$$\sigma_e = \left\{\frac{1}{2}\left[\left(\sigma_x - \sigma_y\right)^2 + \left(\sigma_y - \sigma_z\right)^2 + \ldots \right.\right. \\ \left.\left. + \left(\sigma_z - \sigma_x\right)^2 + 6\left(\sigma_{xy}^2 + \sigma_{yz}^2 + \sigma_{xz}^2\right)\right]\right\}^{0,5} \tag{5}$$

1.3. Computer model

Computer model of the object was implemented in COMSOL Multiphysics environment. The dimensioned model of the object, restrains and a plot of discretization mesh, is presented in Figure 1.

Decision variables in this model are layers thickness values: d_1 and d_2 and their ranges are as follows:

$$d_1 \in [0.2-3]\ \mu m, \qquad d_2 \in [0.2-3]\ \mu m$$

Fixed dimensions of the modelled object elements are as follows: d_3=0.5 μm, d_4=15 μm and d_5=15 μm.
The remaining physical values, which were used in numerical simulation, are presented in Table 1.

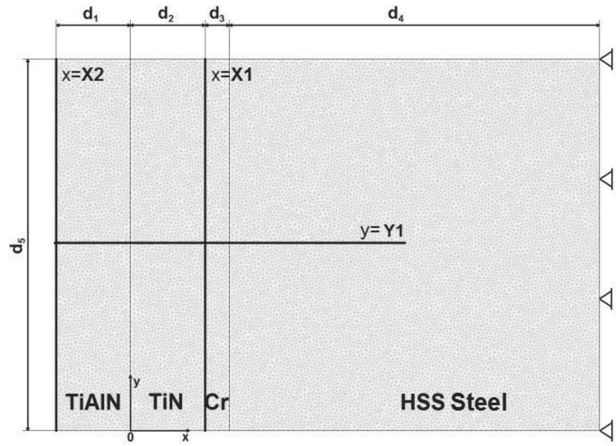

Fig. 1. The schema of the modelled object with its discretization mesh

Table 1.
Material constants used for simulation

Material	Young's modulus [GPa]	Thermal expansion coefficient [1/K]	Poisson's ratio [-]	Density [kg/m^3]
1	380	6.5 10^{-6}	0.23	4700
2	440	9.4 10^{-6}	0.26	5200
3	250	6.2 10^{-6}	0.21	7150
4	210	1.2 10^{-6}	0.30	7860

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:

$$E(x) = E_1 + (E_2 - E_1) \cdot \frac{1}{1 + \exp(-10^7 \beta x)} \tag{6}$$

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:

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

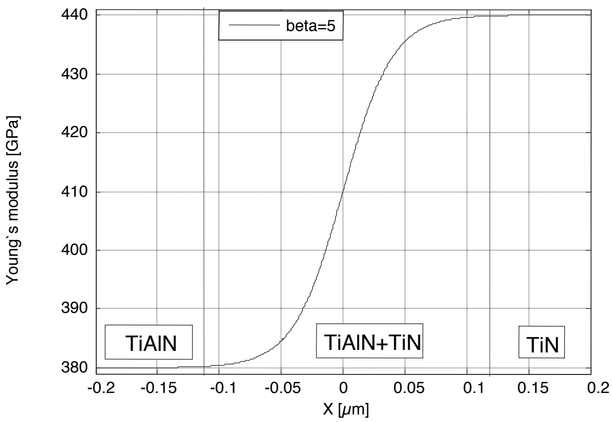

Fig. 2. Flow of Young's modulus transition function, representing its value changes between modelled layers inside coating

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:

$$K_1 = \frac{1}{n}\sum_{i=1}^{n} \left| \sigma_{vm} - \sigma_{ref} \right| \tag{8}$$

where:

n - number of node points on Y1 straight line,

σ_{vm}- Huber Von Mises stress value along Y1 comparative straight line,

σ_{ref} - 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.

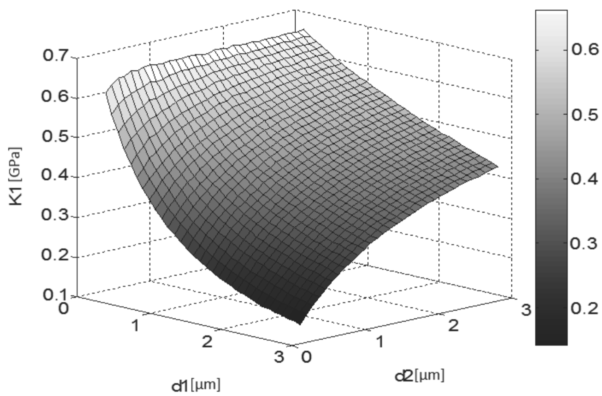

Fig. 3. Objective K_1 as a function of d_1 and d_2 variables

Second decisional objective - K_2 is the minimal stress value σ_y along X1 comparative straight line. Minimal σ_y stress value has negative magnitude, hence minimal stress value - means maximal absolute compression stresses value. Decisional objective K_2 is represented by the equation:

$$K_2 = \min(\sigma_y)_{x=d_2} \tag{9}$$

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.

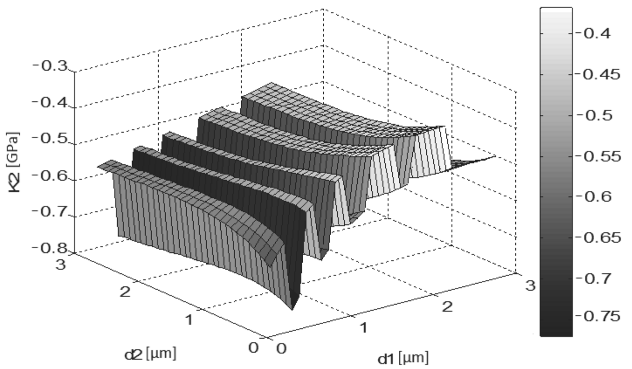

Fig. 4. Objective K_2 as a function of d_1 and d_2 variables

The third decisional objective K_3 is the minimal stress value σ_{vm} along X2 comparative straight line. Decisional objective K_3 is represented by the equation:

$$K_3 = \min(\sigma_{vm})_{x=-d_1} \tag{10}$$

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:

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

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):

$$K_1^{(n)} \to \min,\ \ K_2^{(n)} \to \min,\ \ K_3^{(n)} \to \min \tag{12}$$

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:

$$d \succ d' \Leftrightarrow d - d' \in C \quad C = \{(a_1; a_2) \in R^2 : a_1, a_2 \geq 0\} \tag{13}$$

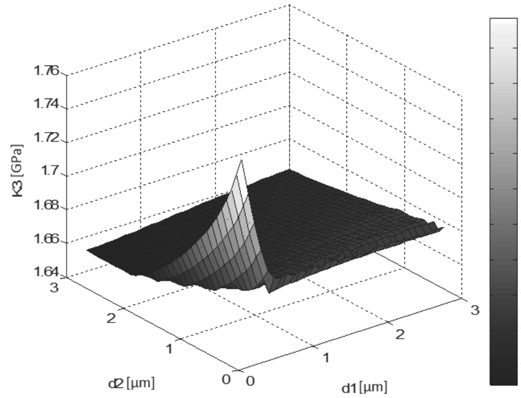

Fig. 5. Objective K_3 as a function of d_1 and d_2 variables

Let K=[K_1, K_2, K_3] 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:

$$K(d^*) \succ K(d) \Rightarrow K(d^*) = K(d) \tag{14}$$

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:

$$d(K_0\ K) = \sqrt{\left(K_1^{(n)}\right)^2 + \left(K_2^{(n)}\right)^2 + \left(K_3^{(n)}\right)^2} \tag{15}$$

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=(K_1, K_2, K_3) 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

Solution	K_1	K_2	K_3	d_1 [μm]	d_2 [μm]
(a)	0.0000	0.7000	0.2429	0.2000	3.0000
(b)	0.9373	0.0000	0.0050	2.9125	0.4625
(c)	1.0000	0.5093	0.0000	2.9125	0.2000
(d)	0.3943	0.3532	0.2418	0.2000	0.9000

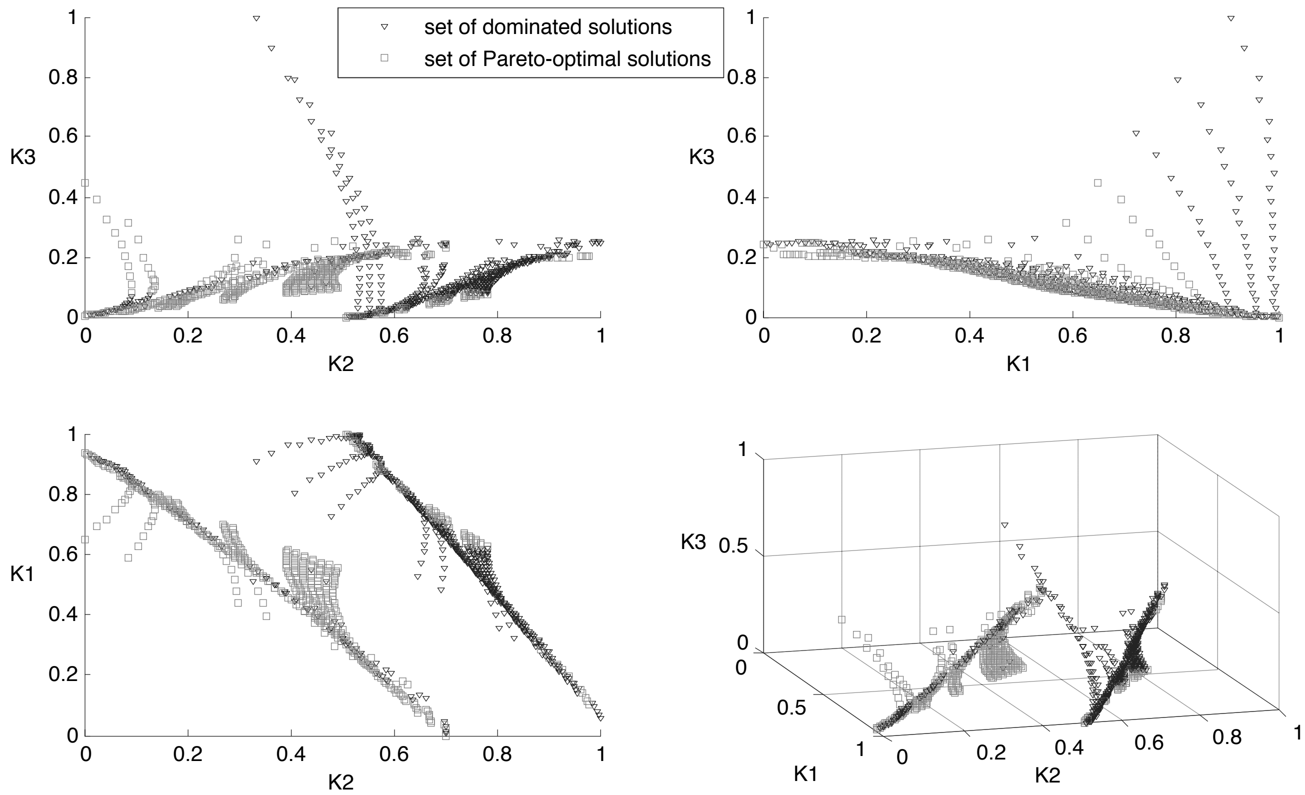

Fig. 6. Dominated and Pareto-optimal solution sets

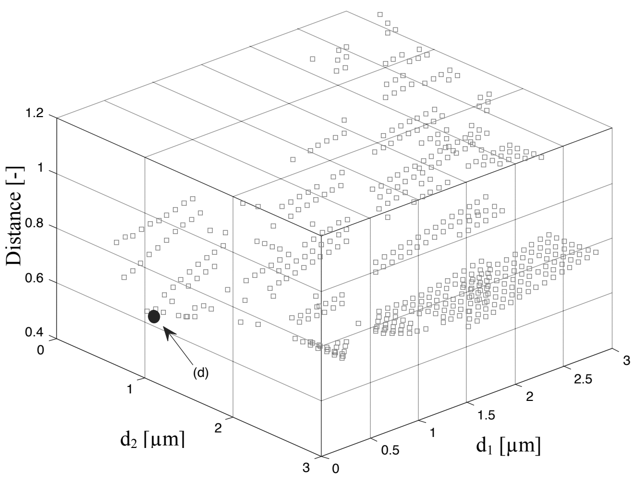

Fig. 7. Functional dpendence of distance values between the points from the objective space $K=(K_1, K_2, K_3)$ and the coordinate system origin $K_0=(0, 0, 0)$

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_3 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.

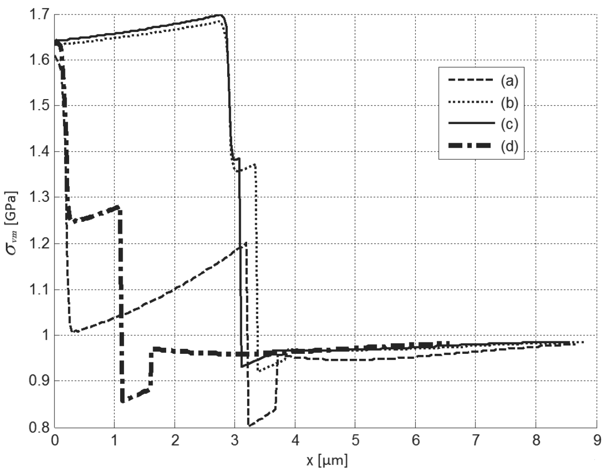

Fig. 8. Huber von Mises stress values versus x variable, along Y1 comparative straight line

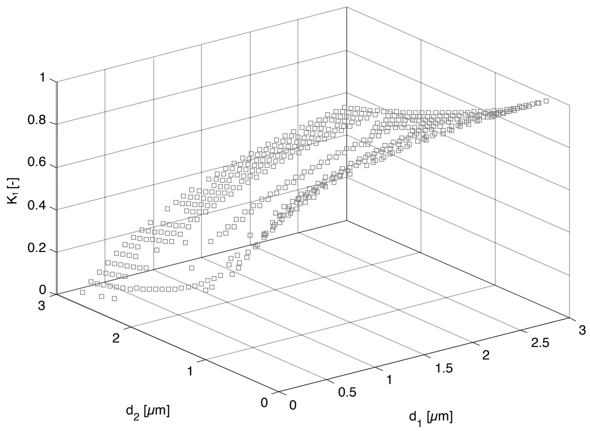

Fig. 9. Functional dependence of objective K_1 value, from decisional variables (Pareto-optimal solutions)

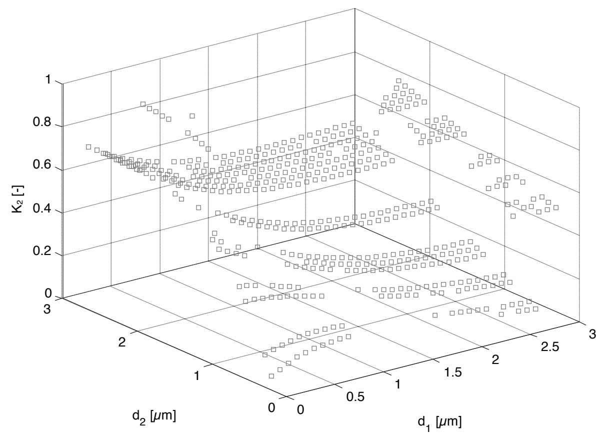

Fig. 10. Functional dependence of objective K_2 values, from decisional variables (Pareto-optimal solutions)

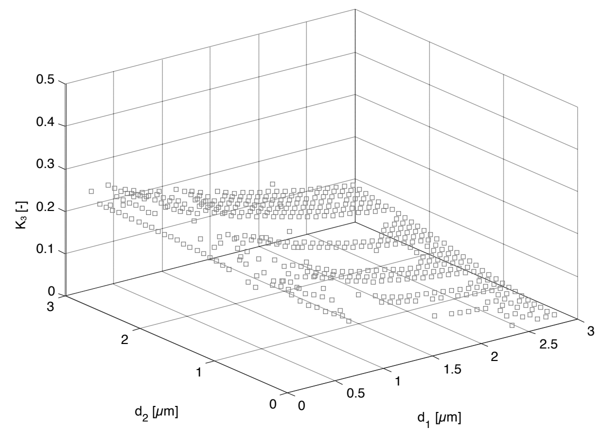

Fig. 11. Functional dependence of objective K_3 values, from decisional variables (Pareto-optimal solutions)

Acknowledgements

The project was partially financed by the European Union within the European Regional Development Fund, 2007-2013.

References

[1] A. Śliwa L.A. Dobrzański, W. Kwaśny, M. Staszuk, 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.

[2] W. Kwaśny, L.A. Dobrzański, M. Król, J. Mikuła, Fractal and multifractal characteristics of PVD coatings, Journal of Achievements in Materials and Manufacturing Engineering 24/2 (2007) 159-162.

[3] R. Valle, D. Leveque, M. Parlier, 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.

[4] R.K. Lakkaraju, F. Bobaru, S.L. Rohde, 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.

[5] A. Śliwa, J. Mikuła, L.A. Dobrzański, FEM application for modelling of PVD coatings properties, Journal of Achievements in Materials and Manufacturing Engineering 41/2 (2010) 164-171.

[6] L.A. Dobrzański, A. Śliwa, W. Kwaśny, Employment of the finite element method for determining stresses in coatings obtained on high-speed steel with the PVD process, Journal of Materials Processing Technology 164-165 (2005) 1192-1196.

[7] A. Śliwa, L.A. Dobrzański, W. Kwaśny, W. Sitek, Finite Element Method application for modeling of PVD coatings properties, Journal of Achievements in Materials and Manufacturing Engineering 27/2 (2008) 171-174.

[8] J. Haider, M. Rahman, B. Corcoran, M.S.J. Hashmi, Simulation of thermal stress in magnetron sputtered thin coating by finite element analysis, Journal of Materials Processing Technology 168 (2005) 36-41.

[9] L.A. Dobrzański, A. Śliwa, W. Kwaśny, The computer simulation of stresses in the Ti+Ti(C_xN_{1-x}) coatings obtained in the PVD process, Journal of Achievements in Materials and Manufacturing Engineering 24/2 (2007) 155-158.

[10] Ł. Szparaga, J. Ratajski, R. Olik, Mathematical modelling and computer simulation of the stresses and strains fields in surface layer of the knife covered with multilayer coating of planning machine to wood treatment, Materials Engineering 176 (2010) 1249-1254 (in Polish).

[11] W. Nowacki, Theory of stiffness, Scientific State Publisher, Warsaw, 1970 (in Polish).

[12] A. Sawicki, Continuum mechanics, Research and Development Institute Polish Academy of Science, Gdańsk, 1994 (in Polish).

[13] R. Bąk, T. Burczyński, Strength of materials with elements of computer aplications, Technical Scientific Publisher, Warsaw, 2001 (in Polish).

[14] M. Kleiber, Introduction to Finite Element Method, Scientific State Publisher, Warsaw, 1989 (in Polish).

[15] J. Kusiak, A. Danielewska-Tułecka, P. Oprocha, Optimization, Scientific State Publisher, Warsaw, 2009 (in Polish).