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On transition functions and nonlinearity measures in gradient coatings

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Analysis and modelling

ABSTRACT

Purpose: In this paper the influence of the shape of transition functions between the single layers of multilayer coating on the final internal stresses states in the coating was investigated. Additionally the degree of nonlinearity and asymmetry of postulated gradient layers was calculated.
Design/methodology/approach: Physical and mathematical models of the layers were created basing on classical theory of elasto-plastic materials. Computer model of the object (coating + substrate) describing internal strains and stresses states in layers, after deposition process, was created using FEM method.
Findings: New concepts of nonlinearity and asymmetry measurability of transition function were introduced. Using predefined measures the dependence between internal stresses fields in postulated class of gradient layers and values of nonlinearity and asymmetry were obtained.
Research limitations/implications: There are an infinite number of possible measures of heterogeneity and nonlinearity of the transition layers. Also there are infinitely many functions with the same measures of asymmetry and nonlinearity, but different mathematical forms, thus a functions of the same measures value form a kind of class of abstraction. So it is convenient to consider specific representatives of the given class and expand the obtained results to remaining representatives which is laborious and ambiguous task.
Practical implications: Proposed measures of gradient layers will become a significant components of the PC software in future, which will upgrade the designing process of hard, wear resistant coatings architecture.
Originality/value: A class of monotonic and asymmetric transition functions, describing continuous physico-chemical material's parameters changes in each layer of K-layered coating was created. Also a new measures of nonlinearity and asymmetry of transition function were introduced.
Keywords: Transition layers; Analysis and modelling; Computational material science; Internal stresses; FEM

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1. Introduction

Subject of computer-aided design of protective layers, is now the object of interest for many industrial and research centers. Recently many industrial and laboratories tests are carried out on multilayer coatings. These layers can be very effective from the perspective of a further increase in fracture toughness, hardness and adhesion. Significant support in this area is commonly used finite element method (FEM), mainly to the prediction of the dynamics of internal stresses distribution and for investigations of temperatures fields evolution. There are a number of publications devoted to measurements and numerical simulations of distributions of stresses and strains occurring in the coatings during and after the deposition process via PVD techniques e.g. [1-8]. Due to the constant modifications of coatings architecture and development in deposition techniques, this subject still remains open. One of the crucial research issues in the area of thin coatings, is a description of the physical mechanisms of the internal stresses arising. In particular more sophisticated mathematical models for the stresses fields time evolution during deposition processes are developed [7-15]. A special interest is paid to gradient layers (Functionally Graded Materials FGM). These layers are the modification of commonly used multilayer coatings, and can be highly effective in order to maximize the adhesion, hardness and thermal stability. The current concept of physical and mathematical description of the transition layers and their possible applications can be found in [16-21]. It should be emphasized the fact that constantly new types of gradient layers are developed and investigated, because of their possible industrial applications. Due to the currently used many types of the transition layers, it might be worth the creation of some standard functions classes and sets of measures, to assess the degree of asymmetry and nonlinearity of graded layers. Described above research issues are extremely important from the perspective of the components creation of the intelligent computer-aided design and optimization of PVD deposition processes [22-24]. A detailed description of the mathematical and physical models of the arising of internal stresses in considered multilayer coatings deposited via PVD techniques can be found for example in [1-7, 16-19].

2. Object

The modelled object is TiAlN/TiN/Cr multilayer coating, deposited on substrate from high speed steel (HSS). The microscopic picture of the architecture of modelled coating is presented in Fig. 1. The thicknesses of TiAlN and TiN layers are 1μm and thicknesses of Cr interlayer and steel substrate fragment are 0,5μm and 5μm respectively. The goal of modelling process is to determine the influence of transition layer shape on the fields of strains and internal stresses in coating layers after deposition with PVD technique.

2.1. Physical model

Physical and mathematical model of internal stresses fields evolution in considered coatings were created on the basis of [1-7, 19,22] and classical theory of elasto-plastic materials [25-27]. Basing on [25-27] stress state is a symmetric, second-order tensor, with six different components. One may transform this tensor to six component vector of the form:

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

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.

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 elasto-plastic body,
- there is a perfect adhesion between the substrate and the Cr layer, and there is a perfect cohesion between layers inside the coating,
- there is a continuous change of the physical and chemical properties(e.g. Young's modulus, Poisson's ratio, thermal expansion coefficient, density), across the coating thickness,
- coating cooling, after its deposition process, was fully radiation process.

Basing on introduced assumptions the mathematical description of layers mechanical properties, the elasto-plastic body model with hardening was used [25-27].

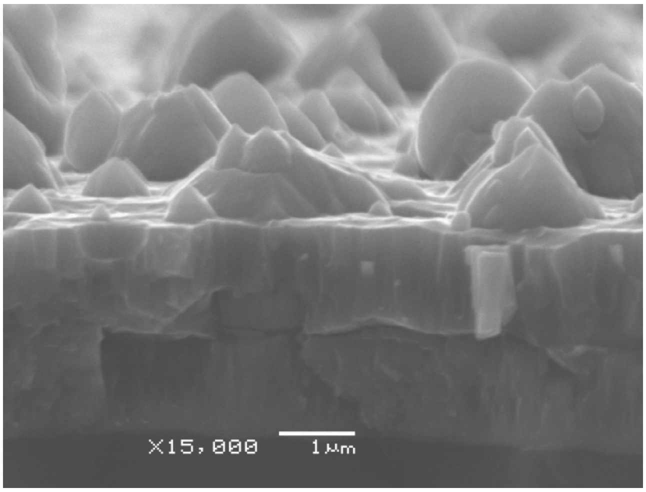

Fig. 1. Structure of TiAlN/TiN/Cr coating

Experimental investigations of gradient character of transition layer occurring between TiAlN and TiN can be done using calotest method. Example of TiAlN/TiN coating with gradient layer deposited via PVD technique is show in Fig. 2.

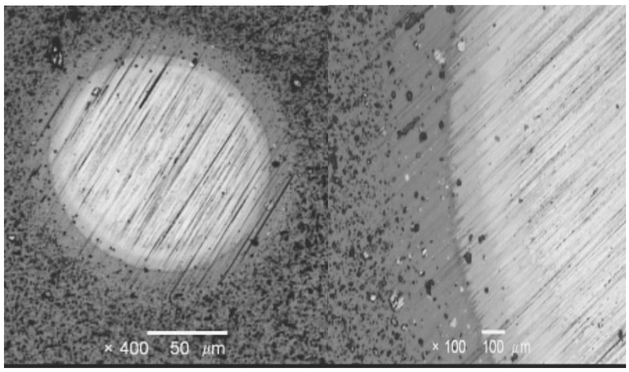

Fig. 2. TiAlN/TiN coating with gradient transition layer

2.2. Computer model

The goal of the numerical simulations was to determine the influence of the shape of transition functions between the TiN and TiAlN layers on the final internal stresses states in the coating. In numerical calculations, because of the object symmetry, the two dimensional strains and three dimensional stresses states were assumed. In order to increase the calculations accuracy a non-homogeneous mesh was used. The schema of the modelled object with mesh, coordinate system and boundary conditions is shown in Fig. 3.

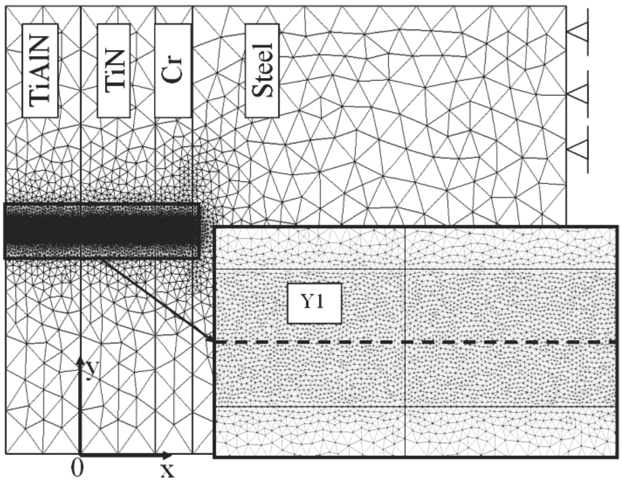

Fig. 3. The schema of the modelled object with mesh

The remaining physical values, which were used in numerical simulation, are presented in Table 1.

Table 1.
Material constants used for simulation

Material	Young's modulus [GPa]	Thermal expansion coefficient [1/K]	Poisson's ratio [-]	Yield strength [MPa]
TiAN	645	7.5 10^{-6}	0.23	6800
TiN	330	9.4 10^{-6}	0.26	4000
Cr	250	4.6 10^{-6}	0.21	320
Steel	210	1.2 10^{-6}	0.30	515

With reference to papers [16,17,19] in which the influence of transition functions on stresses states was investigated, the new classes of asymmetric functions was created. In general postulated functions, describing continuous physico-chemical material's parameters changes in each layer of K-layered coating, are given by the formula:

$$f_{P_{j+1}\to P_j} = P_j + \left(P_{j+1} - P_j\right) \cdot \prod_{i=1}^{N} \left(1 + a_i^{-b_i(x+w_i)}\right)^{-1} \quad (1)$$

where: i=1,2...N and j=1,2...K-1. P_j and P_{j+1} denote physico-chemical material's parameters of j and $j+1$ layer respectively. Parameters w_i, b_i and a_i are responsible for function curvature. In this paper only a subset of transition function (1) is examined. Transition functions used in coating mathematical model have a following form:

$$f_{TiAlN\to TiN} = P_{TiAlN} + \left(P_{TiN} - P_{TiAlN}\right) \cdot \left(a_1^{-5\cdot 10^6(x+w_1)} + 1\right)^{-1} \cdot \left(a_2^{-5\cdot 10^6(x+w_2)} + 1\right)^{-1} \quad (2)$$

where: P_{TiN} i P_{TiAlN} denote physico-chemical material's parameters of TiN and TiAlN layer respectively. The examples of transition functions (2) of Young's modulus for different parameters w_1, w_2, a_1 and a_2 are shown in Fig. 4. Change of functions parameters allow to affects the curvature character. The same types of functions describe directly the change of material's parameters (e.g. Young's modulus, Poisson's ratio, thermal expansion coefficient, density) across the coating thickness.

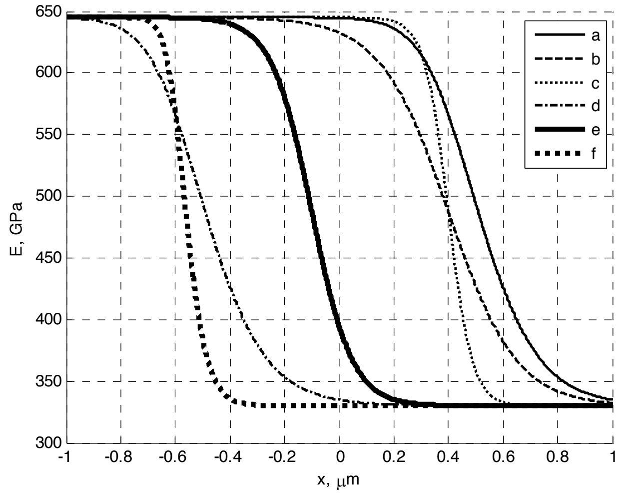

Fig. 4. Courses of transition functions of Young's modulus for different parameters w_1, w_2, a_1 and a_2.

The coefficients of transition functions shown in Fig. 21 are presented in Table 2.

Table 2.
Transition functions parameters

function	a_1	a_2	10^{-6} w_1	10^{-6} w_2
a	5	5	-0.4	-0.4
b	5	100	-0.4	-0.6
c	5	100	0.6	-0.4
d	5	5	0.6	0.6
e	15	25	0.1	0.6
f	100	100	0.6	0.6

Change of physico-chemical properties of TiAlN/TiN gradient layer can be obtained by different technological conditions of deposition, or via control the percentage amount of Al in the coating [7,12,15]. To facilitate analysis of results, the following markings on the ranges of the functions parameters were introduced: $a_{1min}=a_{2min}=5$, $a_{1max}=a_{2max}=100$, $w_{1min}=w_{2min}=-0{,}4\cdot 10^{-6}$, $w_{1max}=w_{2max}=0{,}6\cdot 10^{-6}$.

3. Measures

Abstract theory of measure and measurability has been successfully developed for many years, but this subject is still open because of the new types of measures and its applications in technical and natural sciences. In paper, it was postulated that measure of asymmetry and nonlinearity of the transition layer is a bounded functional defined on a subset of continuous monotonic functions with values in the set of real numbers, i.e.:

$$\hat{M}[f(x)] \to M \in (a;b), a, b \in \mathbb{R}$$

3.1. Asymmetry measure

For the purposes of analysis of transition layer influence on the stresses states in coating the asymmetry measure was postulated in the following form:

$$\hat{M}_1[f(x)] = \frac{f(x_p+h) - 2f(x_p) + f(x_p-h)}{h^2} \quad (3)$$

where point $P = \left(x_p, \frac{E_1+E_2}{2}\right)$.

The M_1 measure is inspired by the definition of the second derivative. The parameter h is related to the length of investigated interval of function value variation. For h approaching to 0 we obtain the value of second derivative in point P. In Fig. 5 an example of transition function E= f(x) for Young's modulus, as well as the calibrating transition functions b(x), c(x) and d(x) were shown. Basing on these calibrating functions a measure M_1 was scaled.

The calibrating functions b(x) and d(x)are given by the formulas:

$$b(x) = \begin{cases} E_1 & for \quad x \in [-d, x_p) \\ \frac{E_1+E_2}{2} & for \quad x \in [x_p, x_p+h] \\ E_2 & for \quad x \in (x_p+h, d] \end{cases} \quad (4)$$

$$d(x) = \begin{cases} E_1 & for \quad x \in [-d, x_p-h) \\ \frac{E_1+E_2}{2} & for \quad x \in [x_p-h, x_p] \\ E_2 & for \quad x \subset (x_p, d] \end{cases} \quad (5)$$

The function b(x) was assumed as a model of maximal asymmetric transition layer and function c(x) as a model of symmetrical one, respectively. The set of M_1 acceptable values was rescaled to the interval [-1, 1]. According to the adopted scaling the value of M_1 measure for calibration function b(x) is 1 $(\hat{M}_1[b(x)] = 1)$, for function c(x) measure M_1 is 0 $(\hat{M}_1[c(x)] = 0)$, and for function d(x) is -1 $(\hat{M}_1[d(x)] = -1)$. In Fig. 6 for a function with parameters *a* from Table 2, a M_1 value as a function of the parameter value *h* was shown.

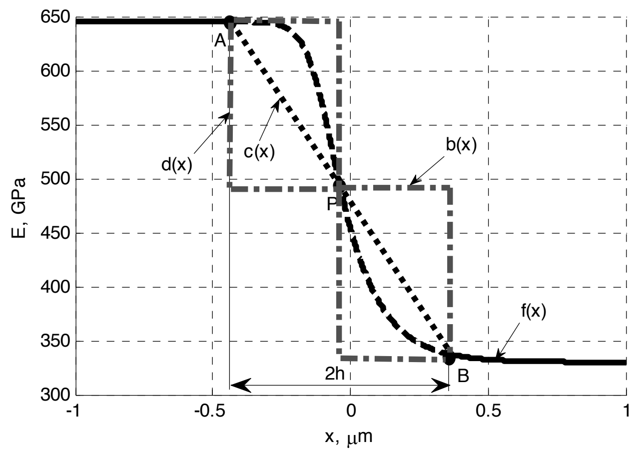

Fig. 5. Courses of transition functions of Young's modulus used for M_1 measure normalization

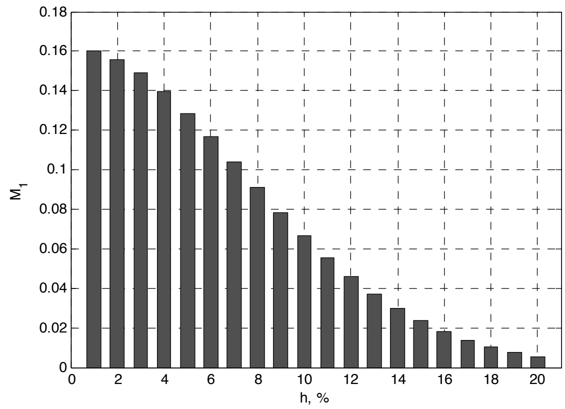

Fig. 6. M_1 value as a function of h parameter

The parameter *h* is expressed as a percentage of the thickness of the TiAlN and TiN layers. For small values of the *h* parameter the local function asymmetry is estimated. Increasing the value of the parameter h corresponds to examination of function asymmetry on wider range of variation, which allows for some kind of averaging the degree of asymmetry. What is more $M_1 \in [-1;1]$, and its sign is directly related to functions convexity character i.e. M_1<0 means concave function, and M_1>0 means convex function.

3.2. Nonlinearity measure

For the purposes of analysis of transition layer influence on the stresses states in coating the nonlinearity measure was postulated in the following form

$$\hat{M}_2[f(x)] = \max_{x \in [x_p-h; x_p+h]} \left(\frac{|A_1 x + A_2 f(x) + A_3|}{\sqrt{A_1^2 + A_2^2}} \right), \quad (6)$$

where A_1, A_2 and A_3 are coefficients of linear function in general form, which goes through points A and B. The idea of M_2 measure is based on the distance d between the transition function f(x) and the straight line passing through the points A and B. In Fig. 7 an example of transition function E= f(x) for Young's modulus, as well as the calibrating transition functions b(x), and c(x) were shown. Basing on these calibrating functions a measure M_2 was scaled.

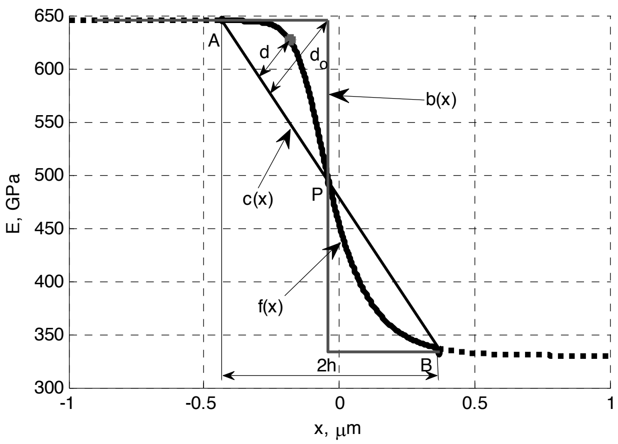

Fig. 7. Courses of transition functions of Young's modulus used for M_2 measure normalization

The calibrating function b(x) is given by the formula:

$$b(x) = \begin{cases} E_1 & for \quad x \in [-d, x_p) \\ E_2 & for \quad x \in (x_p, d] \end{cases} \tag{7}$$

The function b(x) was assumed as a model of maximum nonlinear transition layer, and function c(x) as a model of linear one (constant gradient value), respectively. The set od M_2 acceptable values was rescaled to the interval [0, 1]. According to the adopted scaling the value of M_2 measure for calibration function b(x) is 1 $(\hat{M}_2[b(x)] = 1)$, and for function c(x) measure M_2 is 0 $(\hat{M}_2[c(x)] = 0)$. In Fig. 8 for a function with parameters *a* from Table 2, a M_2 value as a function of the parameter value *h* was shown.

The parameter *h* is expressed as a percentage of the thickness of the TiAlN and TiN layers. For small values of the *h* parameter the local function nonlinearity is estimated. Increasing the value of the parameter *h* corresponds to examination of function nonlinearity on wider range of variation. With the increase of parameter *h* value, the M_1 measure provides a picture of an averaged measure of asymmetry in given interval. M_2 measure informs about the grade of transition function point deviation from the linear trend. It should be emphasized that there are infinitely many functions with the same measures M_1 and M_2 but different mathematical forms, thus a functions of the same measures value form a kind of class of abstract. However, for practical purposes it is convenient to consider specific representatives of the class. Next obtained results can be expanded to remaining representatives (elements) of the class.

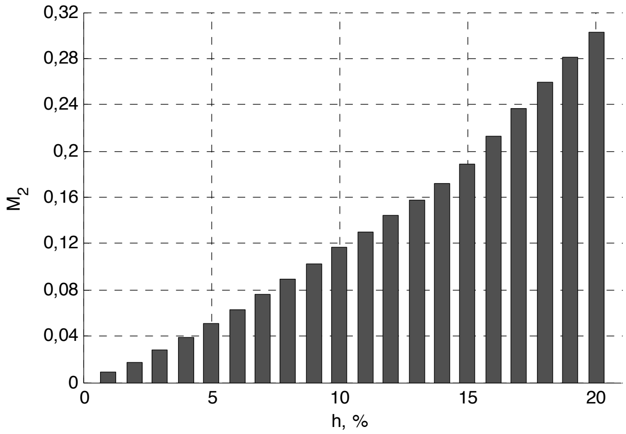

Fig. 8. M_2 value as a function of h parameter

4. Results

The goal of the numerical simulations was to determine the influence of the shape of transition functions between the TiN and TiAlN layers on the final internal stresses states in the coating. In general, the transition function (2) parameters can form the space which can have any finite number of dimensions. In the paper the considered form of transition function (3) is associated with 4-dimensional parameter space. Nonetheless our investigations will be limited to a particular subspace of parameter space i.e.:

$$D = (w_{1min} ; w_{1max}) \times (w_{2min} ; w_{2max}) \times (a_{1min} ; a_{1max}) \times (a_{2min} ; a_{2max}) \subset \mathbb{R}^4 \tag{8}$$

In Figs. 9, 11, 13, 15, 17 and 18 the normal stresses σ_y as a function of x variable (distance from the surface), along Y1 comparative straight line for different subsets of *D* set (8) were shown. Additionally, the values of previously defined measures of asymmetry M_1 and nonlinearity M_2 for the transition functions (2) were computed. For both measures M_1 and M_2 the h parameter was 10%.

In Figs. 10, 12, 14, and 16 the values of measures M_1 and M_2 for different transition functions parameters (a_1, a_2, w_1, w_2) were shown.

In Figs. 19 and 20 M_1 and M_2 values as a function of w_1 and w_2 parameters for a_{1min} and a_{2min} were shown. These figures show measures distributions for transition functions for which normal stresses σ_y as a function of x variable (distance from the surface), along Y1 comparative straight line for different values w_1 and w_2 for a_{1min}, a_{2min} are shown in Fig. 21. It can easily been seen that measures distributions (Figs. 19 and 20) are a quasi symmetrical ones.

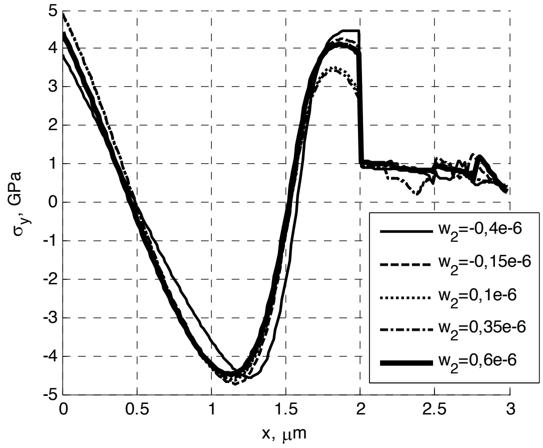

Fig. 9. Normal stresses σ_y as a function of x variable (distance from the surface), along Y1 comparative straight line for different values w_2 for a_{1min}, a_{2min} w_{1min}

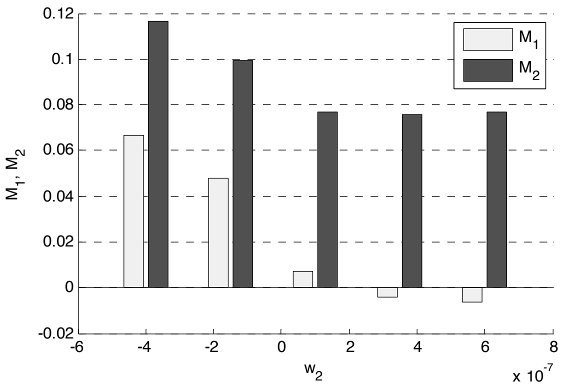

Fig. 10. Values of measures M_1 and M_2 for different transition functions parameters w_2 for a_{1min}, a_{2min} w_{1min}

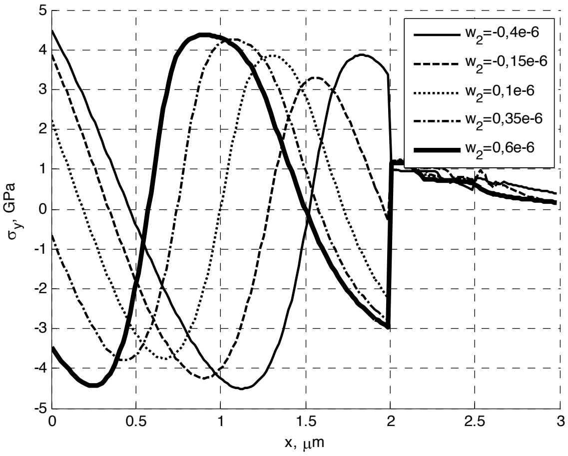

Fig. 11. Normal stresses σ_y as a function of x variable (distance from the surface), along Y1 comparative straight line for different values w_2 for a_{1min}, a_{2min} w_{1max}

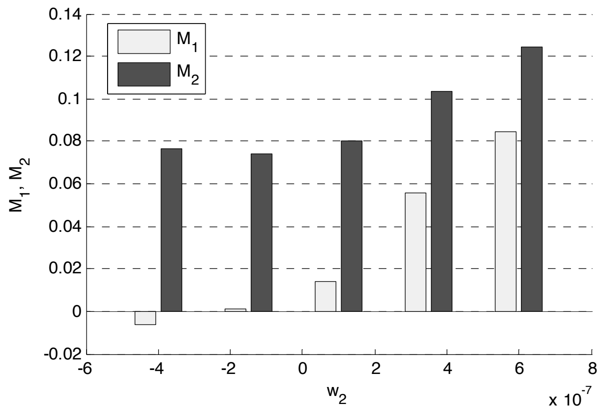

Fig. 12. Values of measures M_1 and M_2 for different transition functions parameters w_2 for a_{1min}, a_{2min} w_{1max}

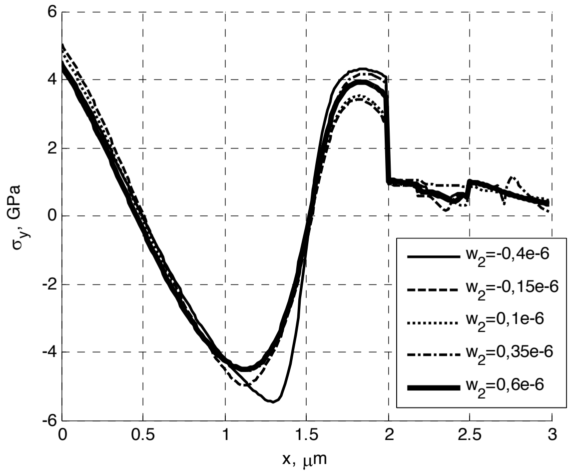

Fig. 13. Normal stresses σ_y as a function of x variable (distance from the surface), along Y1 comparative straight line for different values w_2 for a_{1min}, a_{2max} w_{1min}

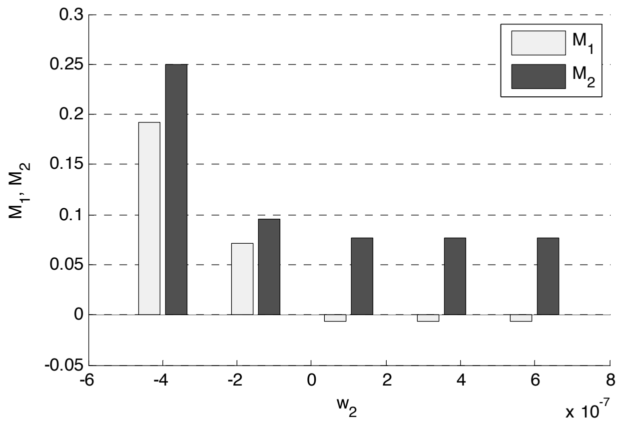

Fig. 14. Values of measures M_1 and M_2 for different transition functions parameters w_2 for a_{1min}, a_{2max} w_{1min}

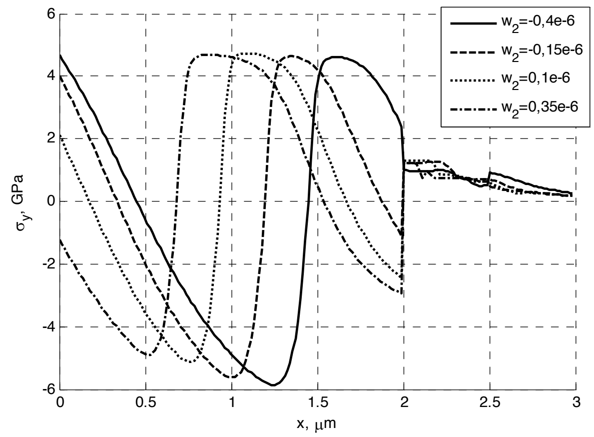

Fig. 15. Normal stresses σ_y as a function of x variable (distance from the surface), along Y1 comparative straight line for different values w_2 for a_{1min}, a_{2max} w_{1max}

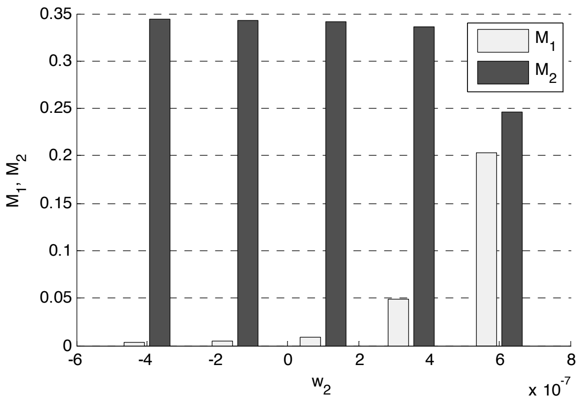

Fig. 16. Values of measures M_1 and M_2 for different transition functions parameters w_2 for a_{1min}, a_{2max} w_{1max}

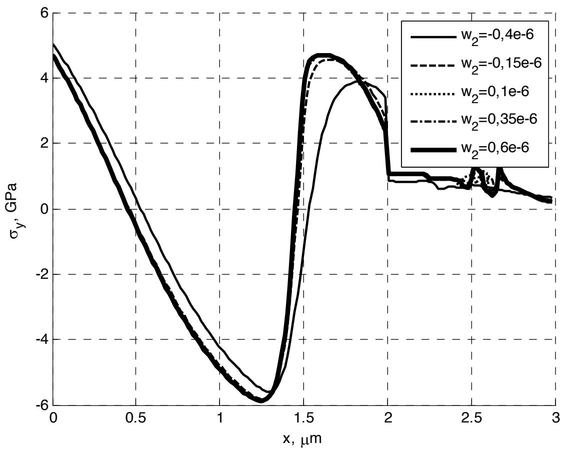

Fig. 17. Normal stresses σ_y as a function of x variable (distance from the surface), along Y1 comparative straight line for different values w_2 for a_{1max}, a_{2min} and w_{1min}

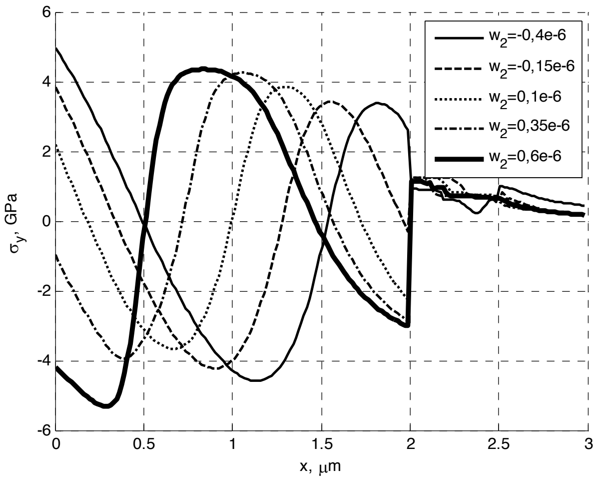

Fig. 18. Normal stresses σ_y as a function of x variable (distance from the surface), along Y1 comparative straight line for different values w_2 for a_{1max}, a_{2min} and w_{1max}

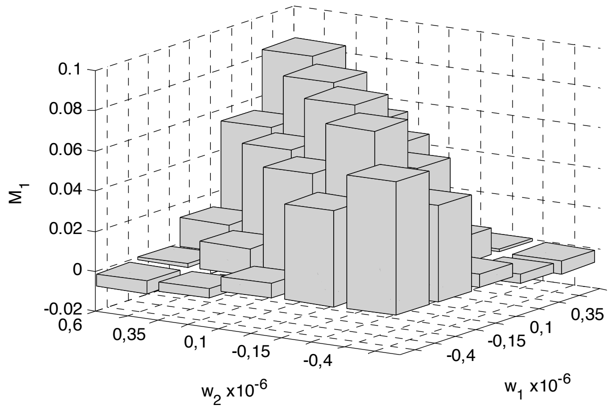

Fig. 19. M_1 value as a function of w_1 and w_2 parameters for a_{1min} and a_{2min}

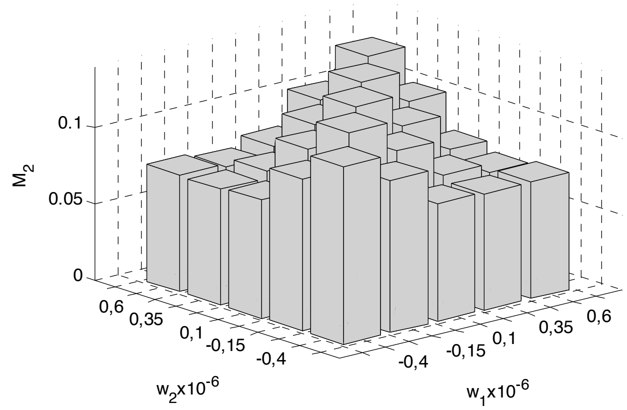

Fig. 20. M_2 value as a function of w_1 and w_2 parameters for a_{1min} and a_{2mi}

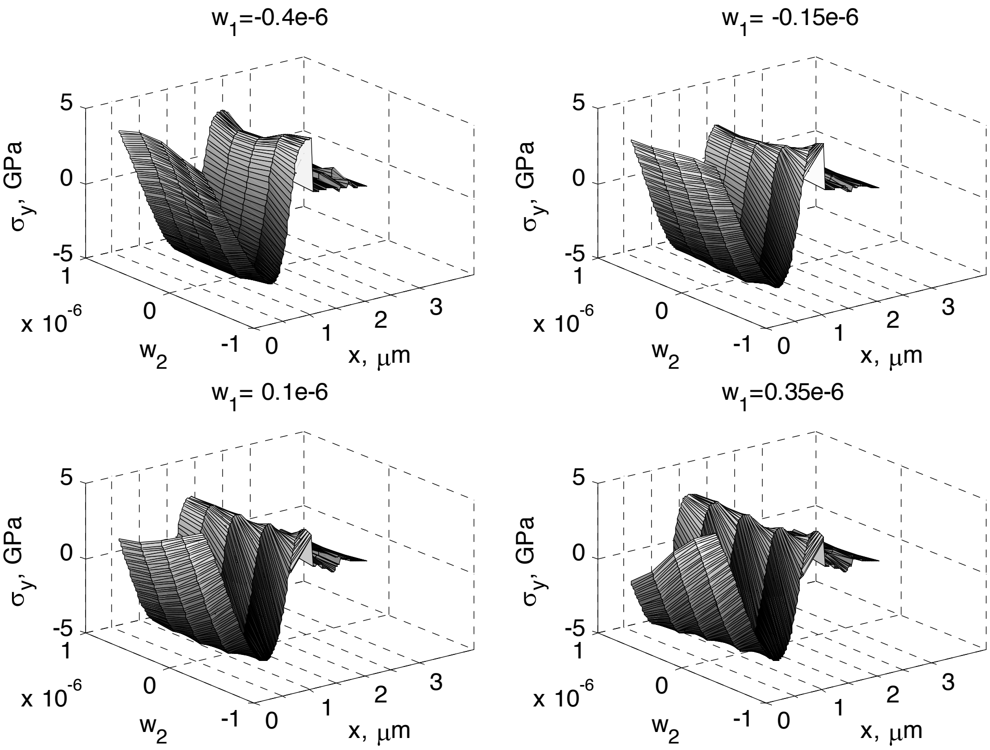

Fig. 21. Normal stresses σ_y as a function of x variable (distance from the surface), along Y1 comparative straight line for different values w_1 and w_2 for a_{1min}, a_{2min}

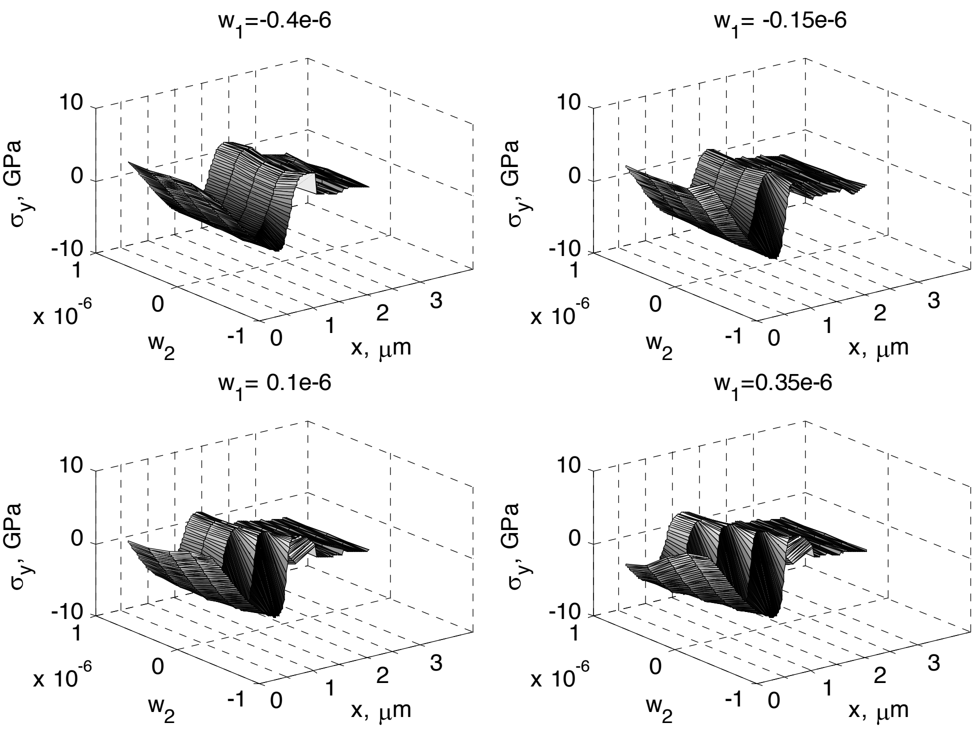

Fig. 22. Normal stresses σ_y as a function of x variable (distance from the surface), along Y1 comparative straight line for different values w_1 and w_2 for a_{1min}, a_{2max}

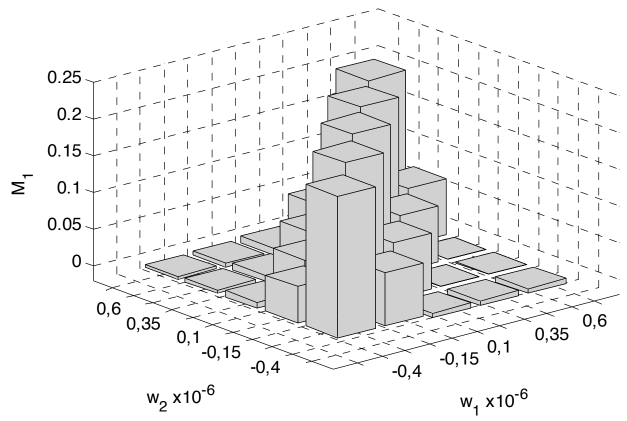

Fig. 23. M_1 value as a function of w_1 and w_2 parameters for a_{1min} and a_{2max}.

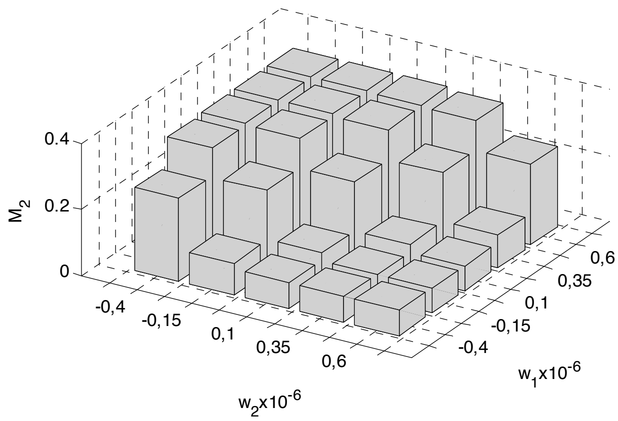

Fig. 24. M_2 value as a function of w_1 and w_2 parameters for a_{1min} and a_{2max}

In Figs. 23 and 24 M_1 and M_2 values as a function of w_1 and w_2 parameters for a_{1min} and a_{2max} were shown. These figures show measures distributions for transition functions for which normal stresses σ_y as a function of x variable (distance from the surface), along Y1 comparative straight line for different values w_1 and w_2 for a_{1min}, a_{2max} are shown in Fig. 21. It can easily been seen that measures distributions (Figs. 23 and 24) are asymmetrical ones.

5. Conclusions

Creation measures of asymmetry and nonlinearity of the transition functions is a step towards creating a universal sets of widely used metrics for functionally graded layers. However, it should be emphasized that, there are an infinite number of possible measures of heterogeneity and nonlinearity of the transition layer. It is intentional to create the largest possible number of different measures and then determine which of the studied types may be used for specific technological applications.

It should be expected that in order to classify functionally graded layers is not possible to create one universal measure. The solution to this problem might be a usage a several measures simultaneously to describe given gradient layer. The proposals of measures can be successfully used in all types of monotonic functions. The creation of a universal concept of cataloging the transition layers is for sure a difficult and highly ambiguous task. It should however be stress the fact that the analytical description specific transition functions may be needed a high number of parameters responsible for curvature of the function. The introduction of asymmetry and nonlinearity measures will certainly reduce the number of used parameters. In the area of functions which do not have an analytical form, for example functions given as an experimental data tables, usage of measures could be a very effective tool for the assessment their degree of nonlinearity and asymmetry. It should be once again emphasized that there are infinitely many functions with the same measures M_1 and M_2 but different mathematical forms, thus a functions of the same measures value form a kind of class of abstraction. However, for practical purposes it is convenient to consider specific representatives of the given class. Finally obtained results can be expanded to remaining representatives (elements) of the class. Natural extension of the carried out investigations will be creation of multi argument measures, which arguments will be for example single nonlinearity, asymmetry and heterogeneity measures. This measure will enable the simultaneous assessment of influence of transition function properties on the global character of gradient layer.

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