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# Strain field analysis in nanoindentation test of gradient coatings

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## ABSTRACT

**Purpose:** In the paper strain distributions within TiAlN/TiN gradient coatings in nanoindentation test were analysed. The main goal was to examine the influence of the type of a gradient layer on strain distributions in the area of the indenter/coating.

**Design/methodology/approach:** For physical modelling purposes Cr, TiN and TiAlN layers were treated as a continuous medium. Basing on this simplification for the mathematical description of the strain states in the coating a classical theory of stiffness was used. Gradient layers were modelled using the conception of transition function which describe continuous physico-chemical material parameters changes in each layer in the multilayer coating. The computer analysis of the strain fields in the coating after deposition process was done vie FEM method.

**Findings:** For a chosen types of gradient coatings the strain distributions in the coating under external loads (nanoindentation test) were calculated. Using created examples of transition functions, the influence of the shape of the function on strain isolines in the area of the indenter/coating was examined.

**Research limitations/implications:** The main simplification which was done during creation of the mathematical model was an assumption that the coating and the substrate are continuous media. This assumption causes that some physical effects occurring during experimental nanoindentation test can not be properly described in a computer model. Also there are numerous mathematical models of contact, so obtained numerical results (strain distributions) strongly depend of the postulated contact model.

**Practical implications:** For a practical implications of the obtained results one should include a mathematical description of the strain states in the nanoindentation test of gradient coatings. The stress and strain fields analysis is extremely important in respect of fracture analysis. It should be also emphasis, that proposed mathematical description of gradient layer using transition function conception is an easy way to represent physical and chemical properties of gradient coating in computer models. The advantage of such a description of gradient layers can be used for example in polyoptimization process of multilayer gradient coatings.

**Originality/value:** The main value of the paper is the comparison study of strain distribution in nanoindentation test of three different gradient coatings represented be three types of transition functions: (a) step function, (b) linear function and (c) modified non symmetrical sigmoidal function.

**Keywords:** Computational Material Science; Gradient Coatings; Transition Function; Nanoindentation Test

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METHODOLOGY OF RESEARCH, ANALYSIS AND MODELLING

## 1. Introduction

Today, the surface modification of materials is growing and it constitutes a vital part of economy and science. One of the most effective ways to modify the surface is a deposition of a thin protective coating using PVD techniques (Physical Vapour Deposition), which are constantly being developed and modified [1,2]. Despite a significant progress in the development of PVD techniques, there are still a number of technological and theoretical issues related to the design, control and optimization of processes. The key issue in this area is a description of the physical mechanisms of internal stress formation inside the coatings, in particular the description of the time and temperature evolution of the stress and strain distributions arising from deposition processes and thermo-mechanical loads. Currently, numerical calculations performed using the Finite Element Method (FEM) constitutes a significant support in the investigation of the abovementioned problems, especially in designing of the coatings architecture and the parameters of deposition processes [3-7], yet because of the numerous types of coatings architectures and deposition processes, this research area is still open. In the field of designing of protective coatings, one should also mention one of the most important and basic diagnostic tests like micro and nanoindentation. A complementary addition to these experimental investigations is an analysis of contact problems in coating/substrate systems using the classical theory of stiffness [8-10] and the FEM. One of the first researchers who used the FEM to design coatings were Komvopoulos [11], Djabella and Arnell [13,14]. They conducted research on contact problems in indenter/coating systems by analyzing elastic stress distributions [11,13,14]. Parallel studies were also conducted on the problems of the contact of the elastic-plastic deformation by Bhattacharya and Nix [15,16] and Komvopoulos (1989) [12]. They demonstrated a correlation between the thickness of the coating, and the formation places and the character of the zone development of a plastic deformation in contact with a spherical rigid indenter. [15,16]. Additionally, Komvopoulos et. al. determined the relationship between the distributions of strain caused by a contact with the cylindrical indenter and the pressure in the contact zone and the load bearing capacity in TiN/Ti systems [12]. From among the studies devoted to the use of FEM to calculate stress fields in the coating due to external loads the papers by Sun et al. [17,18] deserve a special attention. They are a continuation and development of the research carried out by Komvopoulos [11,12]. In particular, Sun et al. investigated the relationship between the thickness of the TiN coating and the mechanical properties of the substrate, and the shape and location of the zone of plastic deformation which arise from the contact with the spherical indenter. Moreover, based on numerical studies, the authors outlined a number of statements relevant to the intelligent designing of coatings on the basis of stress states and a deformation zone analysis. They also investigated the influence of the coating thickness and indentation depth on the degree of distortion of hardness measurements. A mathematical description of contact problems (indenter/ coating systems) is also complementary to the mechanistic studies of coatings cracking under external loads. For example, modeling of the stress state in coatings arising as a result of Rockwell C, F, Vickers and Berkovich testing for an analysis of the initiation and propagation of cracks was investigated among others by Souza, Mustoe and Moore [19-21] and Perez and Souza [22,23]. A continuation and synthesis of the results presented in [19-23] was carried out by Pachler et al. [24]. In particular, they studied the mechanisms of radial and circular cracks in hard ceramic coatings during Rockwell C and F tests. They showed that the circular cracks are caused by large radial stresses which are formed as a result of an insertion of the indenter in the coating. Furthermore, they assumed that a radial crack initiation occurs at the boundary of the indenter's contact with the coating. Additionally, the probability of the occurrence of these cracks increases when the difference in the Young's modules of the coating and the substrate is small, there is a good adhesion of the coating to the substrate, and the coating and the substrate are characterized by a high stiffness. Additionally, they analyzed the micrographs of the coating after the Rockwell C test, noting that the radial cracks are discontinuous and are outside the imprint left by the indenter. Based on the results obtained, they suggested a hypothesis that radial cracks discontinuity was caused by an earlier presence of circular cracks. Using FEM in a computer model of indentation, they confirmed the hypothesis, since according to the results obtained, the maximum value of radial stress responsible for the formation of circular cracks was achieved much faster during insertion indenter than the maximum hoop stress [24]. One of the most recent studies on an analysis of cracks in coatings and modeling the states of stress resulting from the insertion of a nanoindenter in multilayer ceramic coatings is the studies conducted by Zhao, Xie and Munroe [25]. The authors examined the relationship between the type and location of cracks in single and multilayer coatings initiated by external loads. On the basis of the results obtained, they found that for all the types of the coatings investigated, the maximum radial compressive stresses occur in the central zone of contact with the indenter, and the maximum tensile radial stresses occur near the boundary of indenter contact with the coating. On the basis of the stress distributions obtained, they also demonstrated that the equivalent and shear stresses that occur in the multilayer coatings are much lower (about 50%) compared to the stresses in the single layer coatings of the same thickness. Then, assuming that the radial cracks are formed in the contact zone in which the maximum radial and hoop stresses occur, the areas where the probability of appearance of cracks is the greatest were determined. Furthermore, they determined the areas of a high probability of the formation of lateral cracks that arise as a consequence of a high shear stress [25].

Parallel with the studies discussed on the contact issues in homogeneous coatings, studies on coatings with interlayer and transition layers were carried out. One of the first studies on the assessment of the influence of heterogeneous transition layers on the internal stress states in the coating, arising from mechanical and thermal external loads were conducted by Delale and Erdogan [26, 27] and Noda and Jin [28,29]. From among the papers devoted to the study of stress states in a coating with an interlayer, one of the most important ones is the paper by Diao et al. [30]. They conducted a study on the impact of the mechanical properties of the interlayer on stress states in substrate/interlayer/external layer systems, on the assumption that the ratio of the Young's modulus of the external layer to the substrate is constant, and the system is subjected to Hertzian external loads. Using FEM modeling, they determined the functional relationships between the maximum von Mises stresses on the surface of the external layer and the value of the Young's modulus of the interlayer for the different values of the friction coefficient. They also determined the maximum von Mises and shear stress in the interlayer as a function of the thickness of the external layer to the radius of the Herzian contact for different values of the interlayer Young's modulus and for a fixed value of the friction coefficient. Finally, they demonstrated that the interlayers are useful for the purposes of reducing the tensile stresses on the surface, and they can be successfully used to reduce shear stress in the boundary between the coating and the substrate [30]. In later studies, such as [31-35] a certain naming convention became established for transition layers. Namely, it was assumed that if the physico-chemical parameters in the material vary continuously, it belongs to the FGM (Functionally Graded Materials) group. Therefore, substrate/transition layer systems began to be sometimes defined as the substrate/FGM. In turn, transition layer (1)/transition layer (2) systems without any substrate were denoted as FGM1/FGM2 systems. The gradient layer term also began to be used interchangeably with the transition layer term. In the research area of modeling stress states in gradient coatings, the paper by Qianjun Xu et al. [31] is particularly noteworthy. The authors made a comparison of normal and tangential stresses in the boundary between the FGM and the substrate for four types of continuous gradient layers represented by a transition functions: (I) linear, (II) parabolic, (III) square root and (IV) step function. They showed that the layer of type (II) possesses the greatest ability of a stress reduction, whose gradient of the transition function is changing slowly at the surface of the coating, while in the neighborhood of the substrate, it is rapidly increasing. The authors also compiled experimental and simulation results for the substrate/FGM and the substrate/NFGM (Nonfunctionally Graded Materials) systems, and they obtained a good agreement with both types of the results [31].

The present concepts and the modeling methodology of heterogeneous transition layers are contained in the papers by Yongdong et al. [32], Hong-Cai Zhang et al.[33] and Zhang et al. [34]. According to Yongdong et al. [32], one can distinguish four basic types of boundaries between two FGM materials due to the boundary conditions of the transition function and its derivatives: (I) strong discontinuity, (II) weak discontinuity, (III) micro-discontinuity and (IV) continuity. In the mathematical description of physico-chemical parameters, changes between the materials investigated, they used exponential type transition functions. Using the proposed division of boundaries between the two materials FGM1/FGM2 and the three types of external loads applied at the surface FGM1 and FGM2: type 1 tensile stress, type 2 shear stress, type 3 tensile stresses + shear stress, they determined the relationship between the values of stress intensity factors and the exponents of the transition function for different thicknesses of the FGM1 and FGM2 materials. Furthermore, they specified the influence of the type of boundaries on the mechanical properties (such as the crack resistance) of the FGM1/FGM2 coating. The development of the concept of modelling of heterogeneous transition layers in the FGM1/FGM2 materials proposed by Yongdong [32] with new shapes of transition functions and taking into account the transition layer between the two FGM1 and FGM2 materials was the subject of research by Hong-Cai Zhang et al. [33]. They introduced in a great detail the methodology of constructing polynomial transition functions which were used in numerical simulations. Moreover, they analyzed the influence of the transition layer gradient on stress states in the boundary of FGM1/FGM2 under external tensile stresses. Additionally, the authors analyzed the influence of the transition function on stress intensity factors and in the gradient layer between FGM1 and FGM2 with the presence of cracks of a specified width at the boundaries [33]. Finally, the studies by Zhang et al. [34] are also noteworthy. They concern a comparison of internal stress states in monolayers, multilayers and gradient coatings arising from external loads. They also include the modelling methodology of gradient coatings without using any transition functions. The transition layer is approximated by multiple layers for which the Young's modulus varies with the distance from the outer layer [34]. The review of literature is certainly not exhaustive, but it shows a multiple of the problems considered associated with the mathematical description and computer modelling of contact problems in gradient coatings.

The paper presents the results of the research conducted on the influence of the transition layer on strain states in the nanoindentation test of gradient coatings.

## 2. Physical and computer model

The modelled objects were wear resistant gradient coatings composed of TiN and TiAlN and Cr interlayers deposited on a substrate from HSS. Figure 1 shows an example of a spherical metallographic specimen of the gradient coatings modelled.

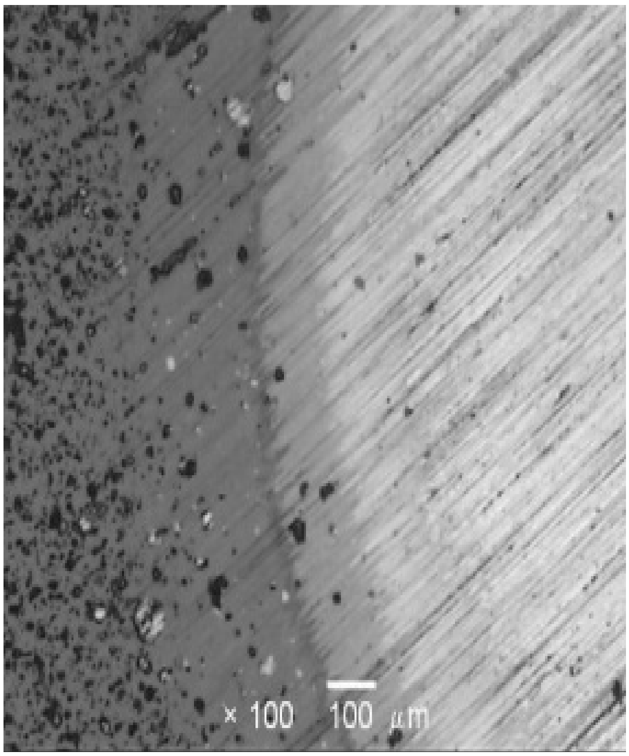


Fig. 1. Gradient coating TiAlN/TiN

The goal of the modelling was to determine fields of strain present in gradient coatings in a nanoindentation test. The following assumptions and simplifications concerning the objects were taken into account during the creation of the model:

- substrate and Cr, TiN, TiAlN layers are treated as continuous media,
- substrates with the coating are assumed to be elasto-plastic bodies,
- there is a perfect adhesion between the substrate and the Cr interlayer, and there is a perfect cohesion between layers inside the coating,
- in the transition layer between TiAlN and TiN material, physico-chemical parameters (the Young's modulus, the Poisson's ratio, the thermal expansion coefficient and density) vary continuously.

The mathematical and physical model describing the formation of strain and stress fields within the coatings considered was created based on the studies [35-38] and the classical theory of elasto-plastic materials [8-10]. A computer model of the objects analysed was implemented in the COMSOL Multiphysics environment. A full characterization of the computational methods used based on FEM is contained in the help documents of the software used. Figure 2 shows a diagram of the objects modelled (coating + substrate) and an indenter with mesh discretization. Coating thicknesses were 2 µm, the thickness of the chromium interlayer was 0.5 µm and the radius and height of the steel substrate cylinder was 50 µm. The radius of the curvature of the diamond indenter was 5 µm, and the indentation depth was 0.2 µm for each of the coatings.
The values of the material constants of the substrate and coatings used in numerical simulations are shown in Table 1.

The change in the parameters of the materials in the transition layer between TiAlN and TiN was modelled using three different types of transition functions. The first type is a step function (Fig. 3a) given by the following formula:

$$E(z)=\begin{cases} E_3 & for\ z\in(50\mu m\ ;\ 50{,}5\mu m) \\ E_2 & for\ z\in[50{,}5\mu m\ ;\ 51{,}5\mu m] \\ E_1 & for\ z\in(51{,}5\mu m\ ;\ 52{,}5\mu m] \end{cases} \tag{1}$$

where: $E_1$, $E_2$, $E_3$ are the Young's modulus of TiAlN, TiN and Cr respectively.

Table 1.
Material constants used for simulation

| Material | Young's modulus [GPa] | Thermal expansion coefficient [1/K] | Poisson's ratio [-] |
|---|---|---|---|
| TiAlN | 645 | $7.5\ 10^{-6}$ | 0.23 |
| TiN | 330 | $9.4\ 10^{-6}$ | 0.26 |
| Cr | 250 | $4.6\ 10^{-6}$ | 0.21 |
| Steel | 210 | $12\ 10^{-6}$ | 0.30 |

The second type is a linear function (Fig. 3b) given by the formula:

$$E(z)=\begin{cases} E_3 \quad for\ z\in(50\mu m\ ;\ 50{,}5\mu m) \\ E_2 \quad for\ z\in[50{,}5\mu m\ ;\ z_A) \\ \dfrac{E_1-E_2}{z_B-z_A}z+\dfrac{E_2z_B-E_1z_A}{z_B-z_A} \quad for\ z\in[z_A\ ;\ z_B] \\ E_1 \quad for\ z\in(z_B\ ;\ 52{,}5\mu m] \end{cases} \tag{2}$$

where: $z_A$ = 51,2 µm, $z_B$ = 52,2 µm, are the boundaries of the transition layer. The third type is a modified sigmoidal function (Fig. 3c), which was postulated in a general form by Ratajski and Szparaga [37]. Its simplified form is it is provided by the following equation:

$$E(z)=\begin{cases} E_3 \quad for\ z\in(50\mu m\ ;\ 50{,}5\mu m) \\ E_2+(E_1-E_2)\left(a_1^{-b_1(z+w_1)}+1\right)^{-1}\cdot \\ \left(a_2^{-b_2(z+w_2)}+1\right)^{-1} \quad for\ z\in[50{,}5\mu m\ ;\ 52{,}5\mu m] \end{cases} \tag{3}$$

where: $a_1 = 5$, $a_2 = 5$, $b_1 = b_2 = 5\cdot10^6$, $w_1 = w_2 = -51{,}5\cdot10^{-6}$.

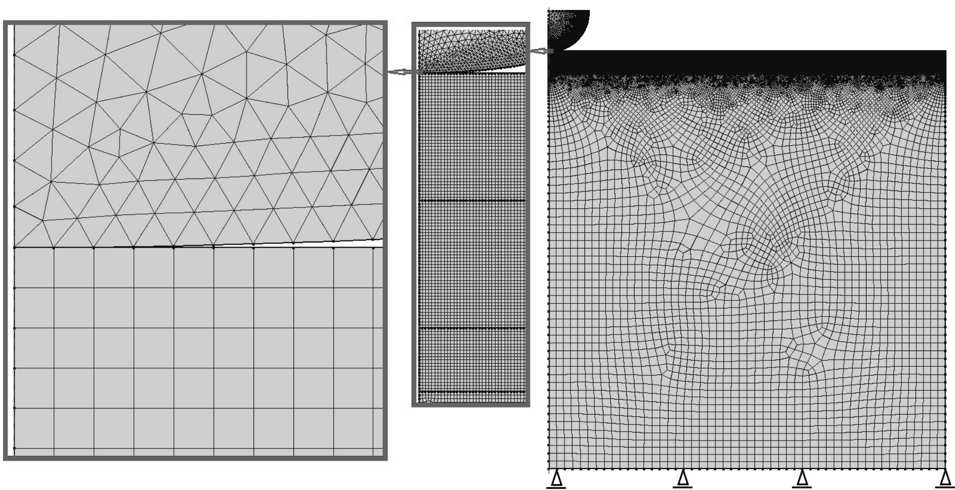

Fig. 2. The diagram of the object modelled with mesh

Analogously, a change to the other parameters of the material, like: the Poisson's ratio, the thermal expansion coefficient and the coating layers' density, were all assumed. It should be emphasized that a change to the parameters of the function (1-3) enables one to control to curvature of the transition function, which directly translates into controlling the participation of each layer in the coating. This fact is extremely important because the representation of the gradient layer using the parameters of the transition function significantly simplifies the potential polyoptimization of the geometry and architecture of gradient coatings.

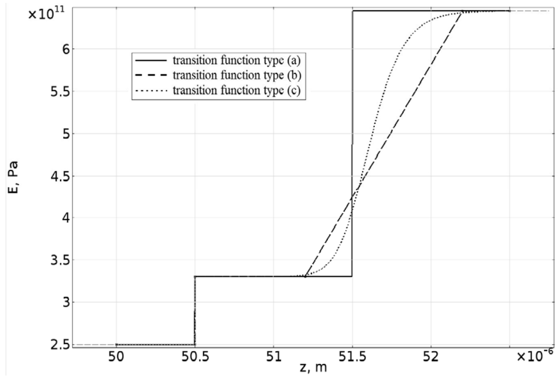


Fig. 3. Dependence of Young's modulus as a function of z coordinate, (a) step function, (b) linear function, (c) modified sigmoidal function

## 3. Results

An analysis of coatings strain states in a nanoindentation test is a key aspect related to the research on the mechanical properties of the coatings. Using the computer model created, strain distributions with isolines were calculated for the studied three types of gradient layers represented by the postulated transition functions. Figures 4-7 present examples of distributions of radial, peripheral, shear and the first principal strain in the of area of the indenter contact with the coating for the (c) type function. According to a review of contact problems, selected strain states carry relevant information related to an analysis of potential cracks.

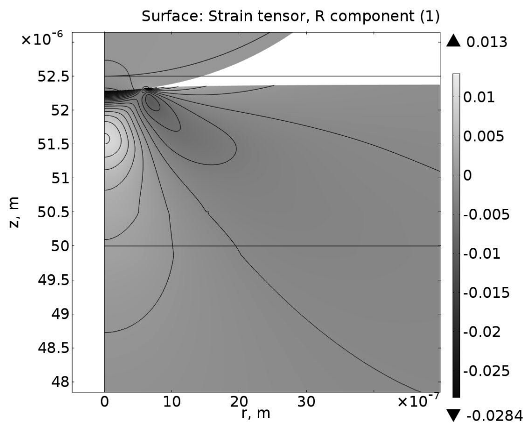


Fig. 4. Radial stain distribution for (c) type transition function

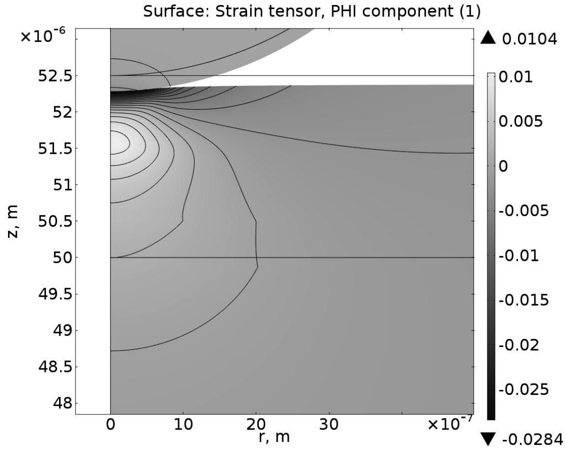


Fig. 5. Peripheral stain distribution (phi component) for (c) type transition function

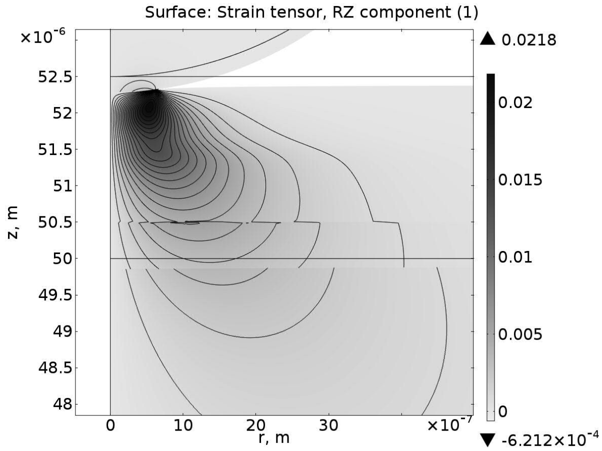


Fig. 6. Shear stain distribution (rz component) for (c) type transition function

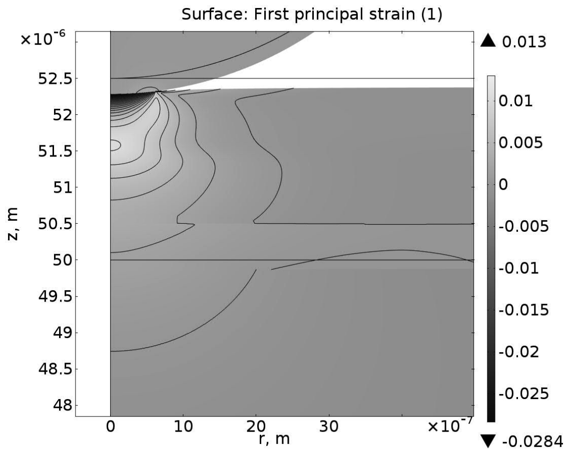


Fig. 7. First principal stain distribution for (c) type transition function

Especially noteworthy are the distributions of radial and peripheral strain (Figs. 4 and 5). In the zone of a direct contact of the indenter with the coating, negative strains are generated, which corresponds to a compressive stress. On the other hand, in the boundary zone between the substrate and the coating, positive strains are formed, which is equivalent to tensile stresses. In shear strain distribution (Fig. 6), it may be observed that the maximum value occurs at a certain depth from the contact boundary. In addition, it can be seen that the contours of shear strain of an equal value are closed. The consequence of this statement is also supported with the research conducted by Zhao et. al. [25], namely that a potential initiation of lateral cracks arises at a certain depth below the contact zone. A comparison of the radial strain value as a function of distance from the top layer for the gradient layers analysed is shown in Fig. 8. It is worth noting that the maximum value of radial strain for each of the analysed transition layers occurs at different depths. This statement is one of the arguments confirming the relationship between the nature of transition function and the mechanical properties of the coating.

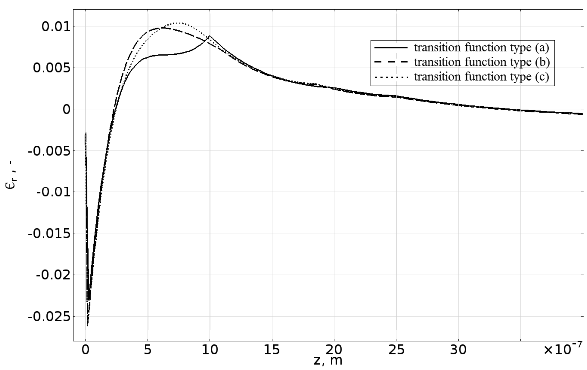


Fig. 8. Radial strain value as a function of distance from the top layer along the symmetry axis for (a), (b) and (c) type transition functions

In order to investigate the influence of the gradient layer on internal strain states in the coating, isolines of equal radial, shear and first principal strains for (a), (b) and (c) type of transition functions were calculated (Figs. 9-14).

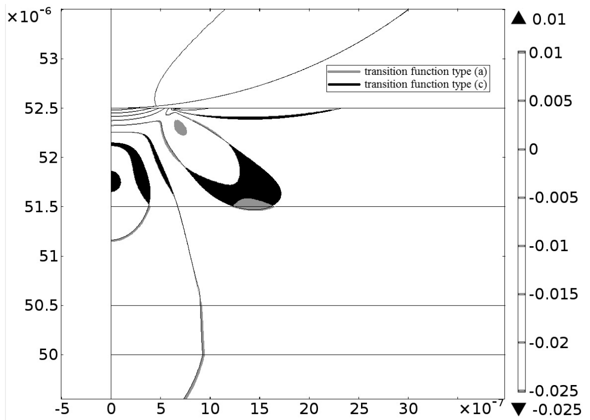


Fig. 9. Isolines of radial strain distributions for (a) and (c) type transition functions

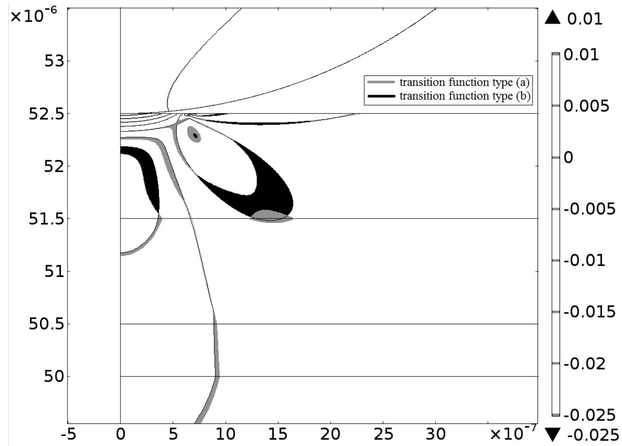


Fig. 10. Isolines of radial strain distributions for (a) and (b) type transition functions

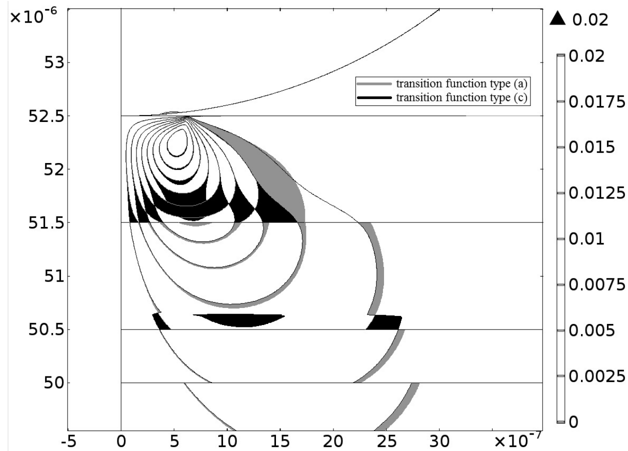


Fig. 11. Isolines of shear strain distributions (rz component) for (a) and (c) type transition functions

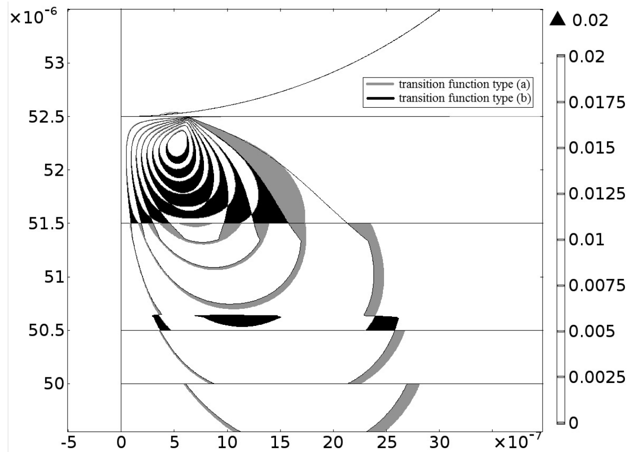


Fig. 12. Isolines of shear strain distributions (rz component) for (a) and (b) type transition functions

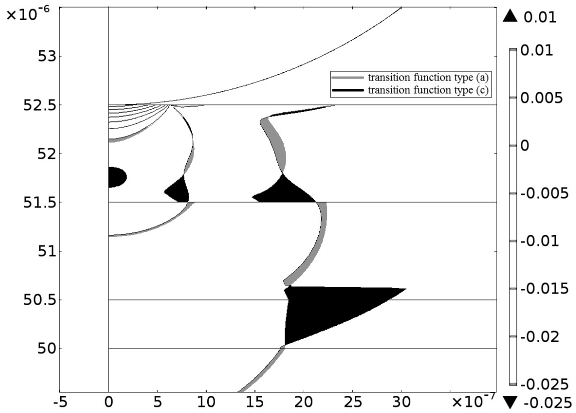


Fig. 13. Isolines of first principal strain distributions for (a) and (c) type transition functions

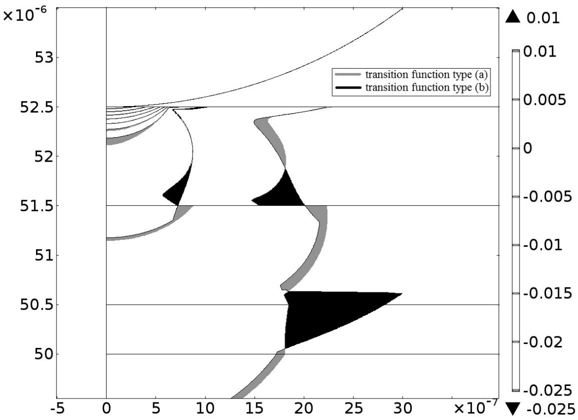


Fig. 14. Isolines of first principal strain distributions for (a) and (b) type transition functions

For the purposes of a comparative study of the coatings analysed, a discrete set of strain values was determined; subsequently, with each of these values, an isoline was associated. An analysis of the influence of the transition function on the strain states was carried out by comparing with each other the shapes of the corresponding isolines for different transition layers. In order to facilitate the analysis, in Figs. 9-14, the following convention was adopted, namely the area dominated by the strain isolines occurring in the coating with the transition layer of the type (a) over the corresponding isolines in the coatings with the transition layer of types (b) and (c) was marked in grey. In turn, the area dominated by those strain isolines that occur in the coating with a transition layer of types (b) and (c) over the corresponding isolines in the coatings with the transition layer of type (a) was marked in black. The main difference in the distributions of the isolines of radial strain between the layers of transitional types (b) and (c), and the transition layer of type (a) (Figs. 9-10) is related to the domination of two particular isolines over others. This domination is caused by the asymmetric nature of the transition functions of type (b) and (c) with respect to the interface between TiAlN/TiN described by the transition function of type (a). A comparison of the isolines distributions of shear strain in coatings with transition layers of type (b) and (c) with the corresponding isolines in coatings with a transition layer of type (a) (Figs. 11-12) provides information about the differences in the shape and location of potential lateral cracks. It should also be noted that some individual isolines present in the coatings with a transition layer of type (b) and (c) dominate simultaneously over several equivalent isolines in coatings with transition layers of type (a) (Figs. 11-12). This fact proves a nonhomeomorphic correspondence between the distributions of the labeled areas of domination. In the distributions of the first principal strain (Figs. 13-14), it is worth to note the presence of three disjoint zones of isolines dominance occurring in the coating with a transition layer of type (b) over isolines present in the coating with a transition layer of type (a), and respectively four zones of dominance for the coating with a transition layer of type c. These zones occur near the boundary between TiAlN/TiN layers (a function of type (a)) and arise as a result of the asymmetry of transition functions of type (b) and (c).

## 4. Conclusions

The main goal of the research carried out was a comparative study of strain distributions within three different TiAlN/TiN gradient coatings in nanoindentation test. In order to analyze the influence of the transition layer on the mechanical properties of the coatings, a comparison of strain isolines was made and the areas dominated by each isoline were determined. It is once again worth to note that some individual isolines present in the coatings with a transition layer of types (b) and (c) dominate simultaneously over several equivalent isolines in coatings with transition layers of type (a) (Figs. 11-12). This does not pose a problem from the point of view of a qualitative comparative study of gradient coatings, but this implies the necessity of an extension of the assessment criteria in order to carry out a strict quantitative comparative analysis. The analysis clearly shows the close relationship between the type of a transition function and the mechanical properties of the coating. However, it should be stressed that in order to draw general conclusions about the influence of the transition function on strain states the study should be extended to include new classes of functions.

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