INFLUENCE OF CHOSEN MICROSTRUCTURE FEATURES ON RESIDUAL STRESS DISTRIBUTION IN FGM SURFACE COATING SYSTEM WITH THE USE OF FEM MICROMECHANICAL RANDOM MODELS

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Abstract

Multilayered coatings established on parts of internal combustion as well as jet engines may be used as TBC systems providing their better thermal-mechanical efficiency, tribological properties, wear resistance and ability to withstand the influence of aggressive media.

The example coating system was established on a beryllium copper substrate and consisted of the NiCr midsurface and TiN external layers. The system was analyzed as a functionally gradient material (FGM) with an assumed linear gradient function of material properties in transition zones between volumes of the pure materials of the substrate, midsurface and the external coating.

The influence of the chosen microstructure features onto distribution of residual stresses was investigated. . These features were: transition zones, porosity and roughness of the external surface of the coating.
Transition zones are the areas at the borders between particular layers of different materials where they are mutually interpenetrated. Different types of porosity were taken into comparisons: evenly dispersed and forming clusters. The 5, 10, 15 and 20% porosities of both of the types were investigated. At last roughness of the coating surface was introduced into the models. All the features were automatically generated with the use of random procedures.

Keywords: *surface coatings, FEM, micromechanical modelling, functionally graded materials, roughness*

1. Introduction

Residual stresses are the problem in the coatings i.e. used as the thermal barriers on surfaces of the elements of such engine pistons and turbine blades or as the anti wear coatings i.e. used on cutting tools. They originate from differences in thermo mechanical properties of joined phases of the coating and substrate materials. Ceramics are elastic and metal substrates are elastic-plastic materials with temperature-dependent characteristics. The residual stress level may be lowered by resulting their redistribution on the way of establishing it as the graded material or functionally graded material (FGM), with several layers with fractions of phases changing by steps or accordingly to the smooth gradient function, respectively.

It was observed that for recognition of the mechanisms responsible for the strength of FGMs the computational methods (FEM among others) are more and more intensively applied.

On the most elementary level, for stress state analysis in the graded materials the law of mixtures is used. Such approach can be used for the elastic systems, for the elastic-plastic systems and also in the Mori-Tanaka method with consideration of phase transformations in the metallic matrix and enclosures.

The law of mixtures, with assumption that in the separate layers the distributions of phases may be treated as practically homogenous – allows to determine the effective properties for the discrete layers of graded material and perform the analysis without necessity of consideration of the real morphology of examined microstructure, with the use of the easy to built mesh consisted of the finite element mesh of a regular shape [1, 3, 5, 6, 8, 10].

On computational way the destruction process of the FGM's may be analyzed and then their properties as well as parameters of technological process of fabrication may be consciously optimised [9].

Analysis of the graded materials may be also performed with the use of realistic or quasi-realistic microstructure geometries. The quasi-realistic geometries may be obtained on the way of generation of domains for the particular material phases. Then the effects of influence of variety of the spatial distributions of the phases onto thermomechanical properties of nonhomogeneous microstructures may be considered. There may be found methods that do not need formulation of assumptions concerning physical and mechanical properties of the particular layers. There are various hybrid approaches, i.e. with the use of so called the Voronoi finite elements, geometry of which describes particular domains and is obtained on the way of Dirichlet's tessellation [2, 7].

3. Models used for the comparative numerical study of a surface coating

A TiN surface coating on the beryllium copper substrate, with a NiCr interlayer, was taken as an example. Such a material system was destined for the use in a pull broach construction.

The three models of TiN surface coatings on the beryllium copper substrate with NiCr interlayer between them were investigated.

Material properties are presented in the Table 1. There was assumed the volume of each material in each model was the same. The same were boundary conditions and the thermal load $\Delta T = -500$ K.

Tab. 1. Material properties

		Beryllium Copper substrate	NiCr interlayer	TiN* coating
E	GPa	130	220	600,00
ν		0,3	0,29	0,250
α	e^{-6} K^{-1}	16,7	11,7	9,4
E –Young's module, ν –Poisson ratio, α - thermal expansion coefficient, * in unporous state (Bull et al. [4])				

The study was performed to examine what are the consequences to the calculated stress distributions when different types of models are used, with different level of simplifications.

The sets of models, which are used in the study:

Model A – transition zones are simulated as multilayered, graded materials,

Model B – transition zones are simulated micromechanically as FGMs and material properties are defined randomly in a grid which consists finite elements of regular square shape,

Model C – porosity effect in the TiN layer is introduced and simulated micromechanically, (C-1: porosity is homogeneous, generated with restrictions to the effects of clustering and joining of pores into voids of larger dimensions; C-2: clustering and joining of pores are allowed),

Model D – roughness of external surface of the TiN layer is introduced and simulated micromechanically.

General assumptions are as follows:

- the same type of finite elements mesh, the same boundary conditions and the same volumes of materials - are retained in all the models,

- in all the models, properties of the TiN are taken like for unporous material (Tab. 1.) and porosity of this layer is simulated micromechanically in the Model C and D,
- in the Model D a roughness of external surface is introduced additionally.

In the Model A (Fig. 1) there were introduced transition zones between the substrate and NiCr layer as well as between NiCr and TiN coating. These areas were built of the same number (20) of sub layers of the same thickness. Material properties in these areas were changed step by step from one sub layer to another accordingly to the linear function, from beryllium copper to NiCr and from NiCr to TiN. The system modelled in such a way may be treated as graded material. There was assumed that materials in all the layers and introduced sub layers are homogenous. Model A doesn't take into consideration such microstructure features like boundaries roughness between the substrate NiCr and TiN layers, interpenetration of materials of neighbouring layers, porosity, voids, micro cracks or roughness of external surface of the coating.

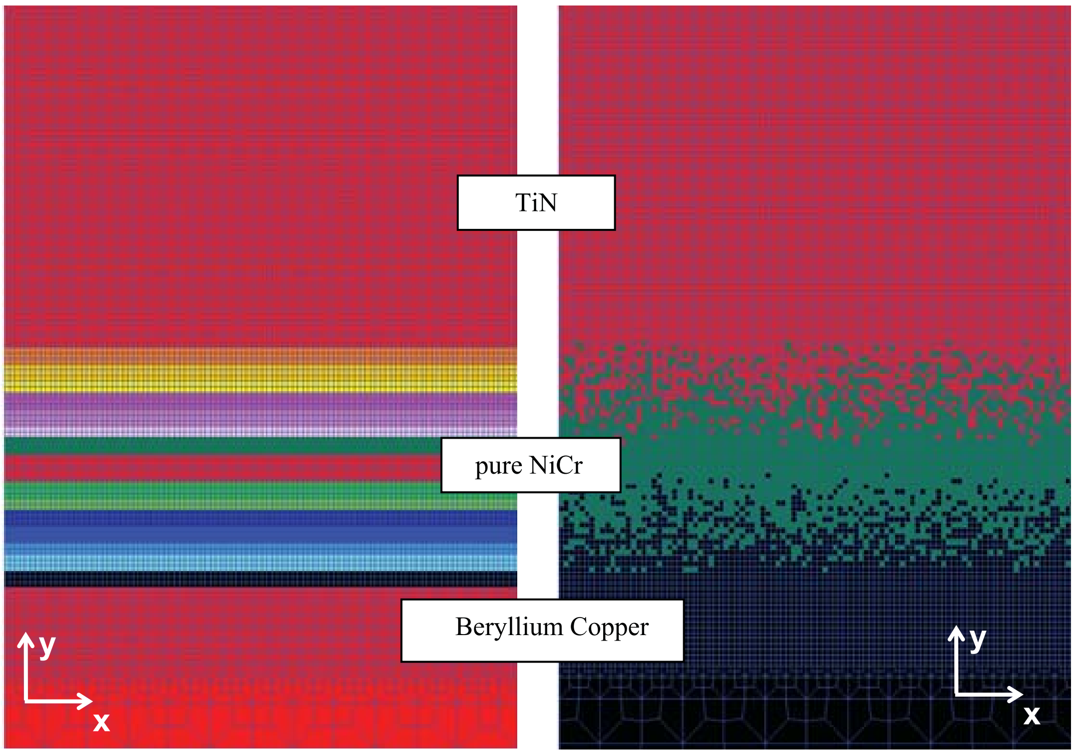

Fig. 1. Model A - transition zones as graded multilayered materials

Fig. 2. Model B - transition zones as functionally graded materials simulated micromechanically

In the Model B (Fig.2), transition areas of the same thicknesses are simulated micromechanically as functionally graded materials, with the same linear gradient functions of material properties like in the Model A. In the grid of material domains, material properties are defined in a random way. The linear gradient function of averaged change of material properties in the depth direction is achieved on the way of changing of probability distribution during the drawing of the material in particular domains.

Model B takes into consideration interpenetration of materials of neighbouring layers, but it still doesn't simulate such microstructure features like porosity, voids, micro cracks, etc.

Thickness of the pure NiCr layer remained the same like in the Model A.

In the Model C porosity was introduced into the model with the use of micromechanical approach. Random definition of pores locations was achieved in 2 ways: with (Model C-1) and

without (Model C-2) restriction of the effect of clustering of pores (possibility of getting close and joining) (Fig. 3, 4).
At last Model C-1 and C-2 were modified by introducing into them a roughness of external surface (Fig. 7, 8).

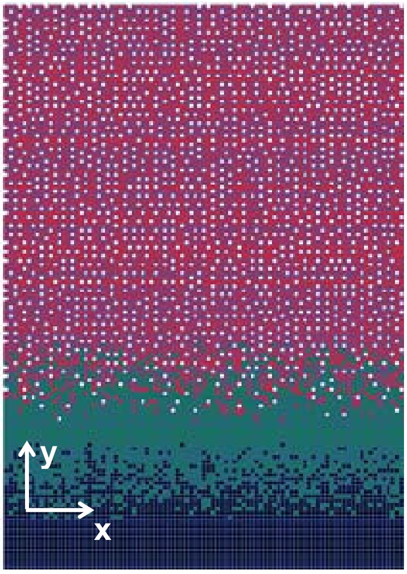

Fig. 3. Model C-1: pores locations randomisation with restriction of clustering effect – an example for 20% porosity

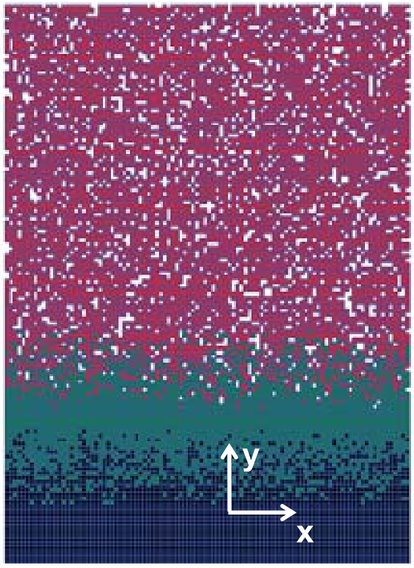

Fig. 4. Model C-2: pores locations randomisation without restriction of clustering effect – an example for 20% porosity

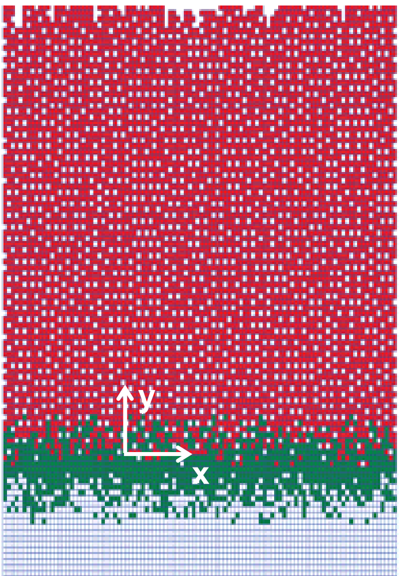

Fig. 5. Model D-1: pores locations randomisation with restriction of clustering effect – and a roughness of external surface introduced – an example for 20% porosity

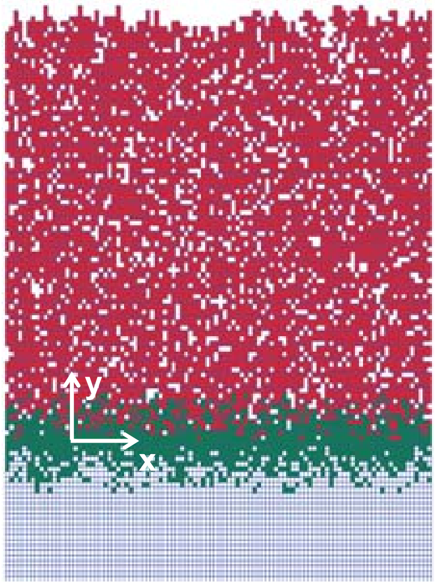

Fig. 6. Model D-2: pores locations randomisation without restriction of clustering effect –and a roughness of external surface introduced – an example for 20% porosity

4. Results and discussion

Model A doesn't take into consideration such microstructure features like boundaries roughness between the substrate NiCr and TiN layers, interpenetration of materials of neighbouring layers, porosity, voids, micro cracks, etc. – so it is still not able to produce non zero values of the σ_y residual stress component. The stress component σ_x distribution is represented as black line in the figure 7.

Model B, as the first one from the presented models, takes into consideration interpenetration of materials from the substrate, interlayer and the coating. Such a model is able to produce non-zero values of the residual stress component, but only in the transition zones (Fig. 7). In the areas of homogeneous materials values of the σ_y residual stress component still remain zero.

Figure 7 presents results for the Model A and B as the product of scanning in search of extreme values of σ_x in function of depth counted from the free surface of the coating. Micromechanical modelling of interpenetration of materials in the transient zones, which was performed in the Model B shows the microstructural effects. In the transient zone that is modelled micromechanically, interpenetrating material domains act like stress concentrators, causing strong oscillations around the average value counted for the particular depth.

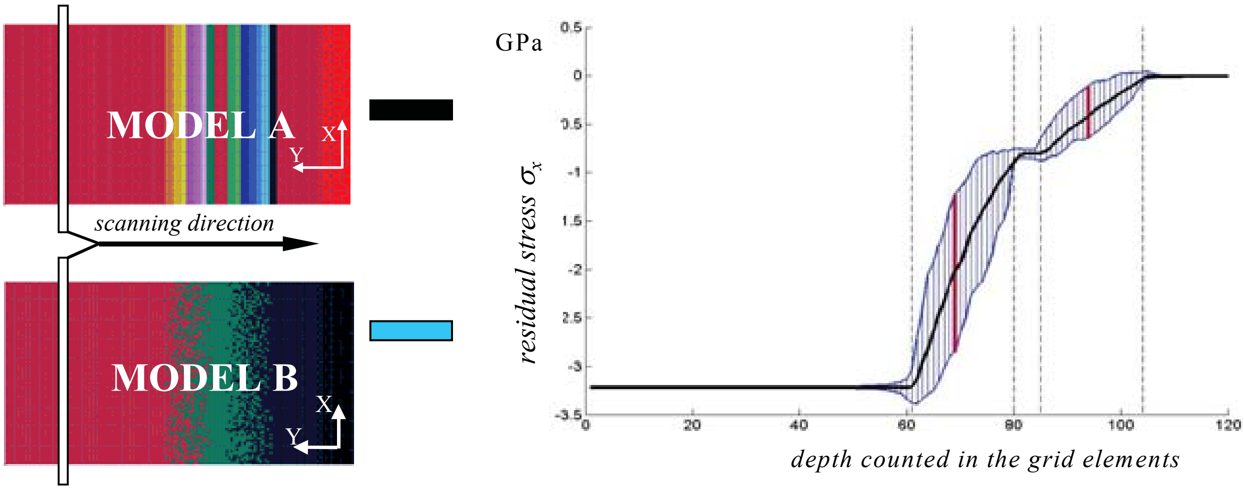

Fig. 7. Comparison of Model A and B – results of scanning in search for extreme values of σ_x stresses in function of the depth (counted in grid element layers, from the free surface of the coating)

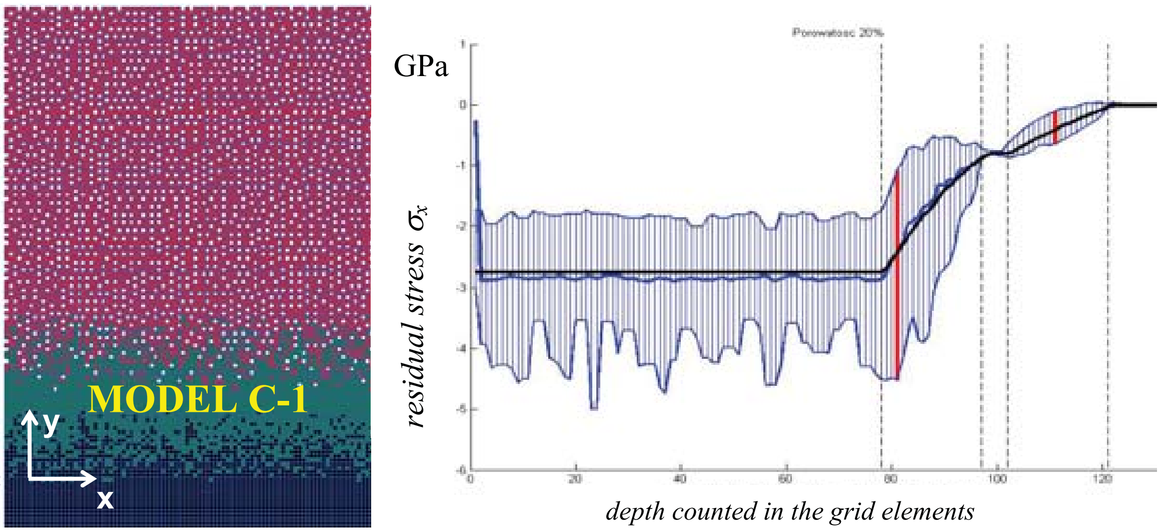

Fig. 8. Model C-1: range of σ_x stress values variations in the coating – randomisation of pores locations with restriction of clustering and joining effect

In the series of Models C-1 where the clustering effect is restricted and the effect of joining of pores is fully eliminated, the ranges of σ_x stress component values oscillations are presented in figure 10 in comparison to those obtained from the Model A (showed as the smooth line in black).

As the clustering effect is not fully eliminated, the lower range of oscillations is affected by separate deviations.

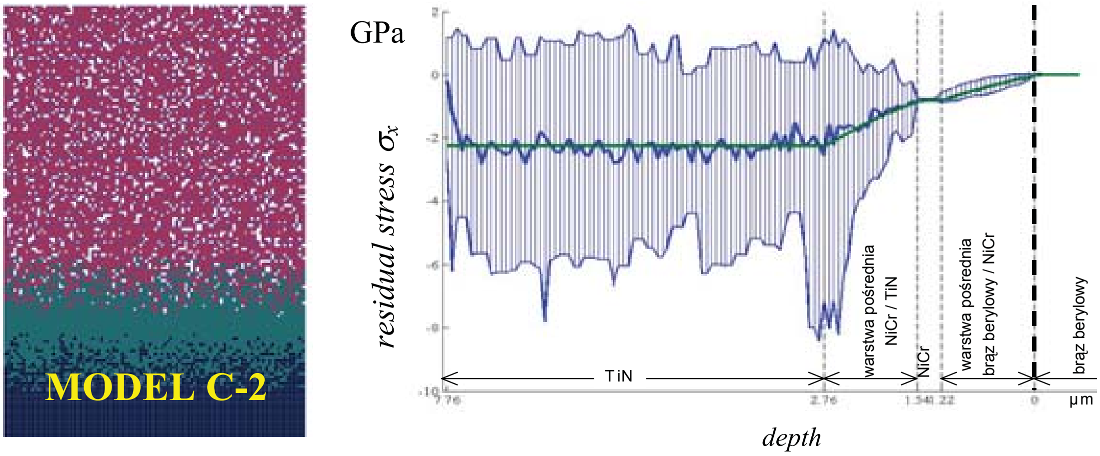

Fig. 9. Model C-2: range of σ_x stress values variations in the coating – randomisation of pores locations without restriction of clustering and joining effect

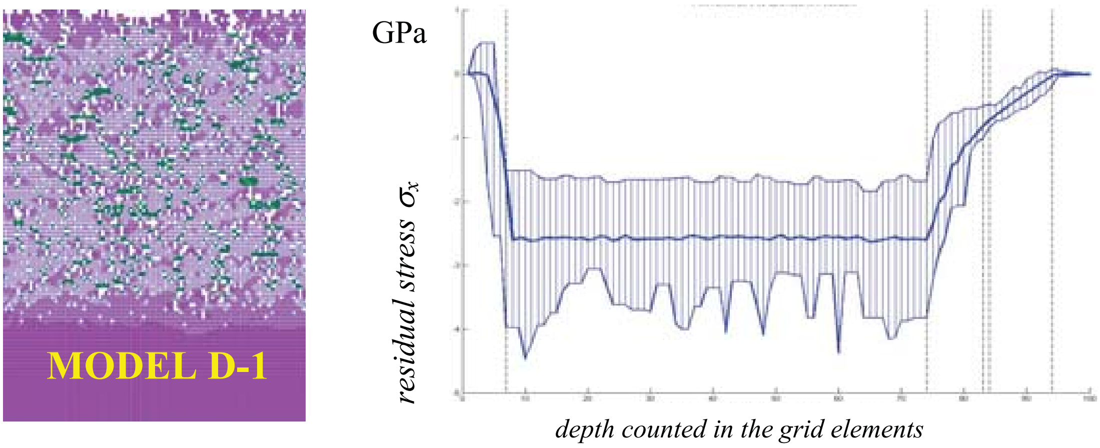

Fig. 10. Model D-1: range of σ_x stress values variations in the coating – randomisation of pores locations with restriction of clustering and joining effect and simulation of a roughness of external surface introduced

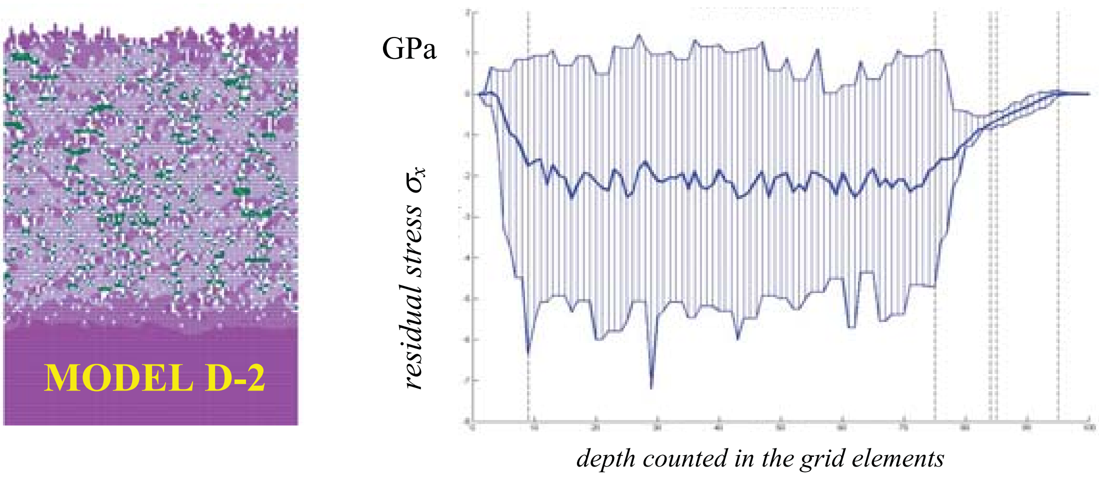

Fig. 11. Model D-2: range of σ_x stress values variations in the coating – randomisation of pores locations with restriction of clustering and joining effect and simulation of a roughness of external surface introduced

In the Model C-2 clustering effect is not restricted and joining of pores into voids of larger dimensions is allowed. This causes much stronger oscillations of σ_x around the average value than in the Model C-1 and the average value is moved into tensile direction, but still remains negative.

Oscillations are strong enough to change locally the sign of stress value: in the coating, were the clustering and joining effect is allowed, tensile stresses originate and they may be strong enough to initiate microcracking. Unless the average value moves into tensile direction, oscillations are strong enough to expand their range to reach greater compression values than in the Model C-1. This may originate crushing of the material at internal free surfaces of voids obtained in the way of joining of smaller pores.

Models D-1 and D-2 were obtained from Models C-1 and C-2 respectively, by introducing a simulation of external surface. The difference in residual stress sx ranges is visible clearly in case Models D-1 and C-1. In both of the models stresses are compressive in the inner area of TiN layer. In the Model D-1 roughness of the external surface cause change of stress value: the average goes to zero, but locally stresses reach tensile values, what can increase intensity of wearing process. In the Model D-2 the effect of roughness is dominated by phenomena of clustering and joining of small pores into bigger voids, but may help in initialisation of cracking process at the external surface, which may cause coating crumbling.

5. Conclusions

The results obtained from micromechanical models of surface coatings treated as graded or FGM materials with the linear function of material phase volume fraction variation, show out the necessity of consideration in numerical simulations mechanisms based on microstructure effects like development and joining of microcracks as well as the effect of presence and nucleation of the voids (on the way of plastic deformations), porosity, interpenetrating and mixing of materials.

Micromechanical simulation of porosity in the TiN layer causes that the average value of residual stress σ_x moves into tensile direction (in comparison to the models with no porosity simulation), but the clustering of pores effect is much more visible and causes strong local increase of compression.

Simplified models, which may be forced in macro scale by limitations in degrees of freedom available on the computer system, should be used very consciously. Simulations of microstructural effects in the area of surface coating are strongly recommended: the comparative study presented here shows out that the results of micromechanical calculations are affected locally too strong to be excluded from considerations.

Simplifications of numerical models passing over microstructural features (like in the Model A) may lead to improper conclusions. The clustering phenomenon strongly affects results. It can be observed that after micromechanical simulation of pores in TiN layer, the average value of residual stress σ_x in this area moves into tensile direction, but the clustering of pores causes that the absolute value of compression arises locally much stronger.

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