COMPARATIVE STUDY OF A FEW FEM MODELS OF A SURFACE COATING SYSTEM

Wiesław Szymczyk

Military University of Technology, Faculty of General Mechanics
Kaliskiego Str. 2, 00-908 Warsaw, Poland
e-mail: w.szymczyk@wme.wat.edu.pl

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 an ability to withstand the influence of aggressive media.

A comparative review of a few different FEM models of a surface coating system is presented which can be used for the needs of designing improved parts of engines. The 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 graded as well as functionally gradient material (FGM) with an assumed gradient function of material properties.

The more advanced models use a micromechanical technique of modeling which enables consideration of microstructure influence on the residual stress distribution. They contain transition zones between the pure material volumes where the material properties change accordingly to the linear gradient function. Simulations of microstructural effects in the area of surface coating are strongly recommended. The results of micromechanical calculations are affected locally too strong to be excluded from considerations.

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

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 optimalized [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].

2. FEM micromechanical modeling of FGM coatings

In preliminary tests upon the establishing the method of the FEM simulation of ceramic surface coating treated as a FGM – the functionally graded material, the numerical micromechanical model (Fig. 1) was used for investigations in micro scale. The model is a microscopic part of an infinite half space.

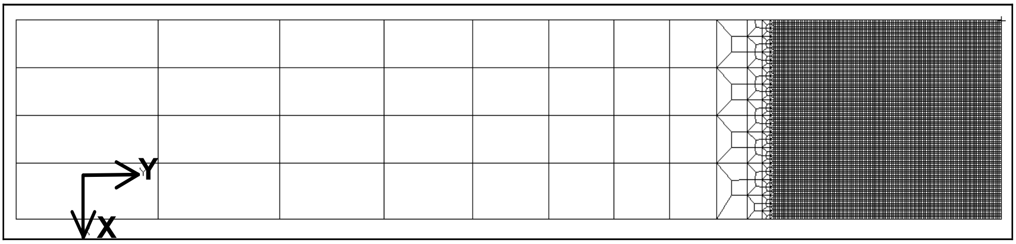

Fig. 1. The FEM model for of simulations FGM structures

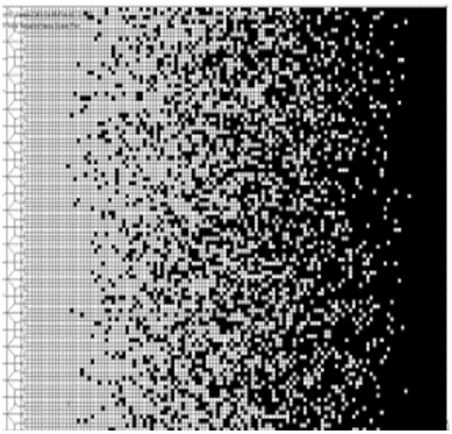

Fig. 2. The zone with linear change of fraction of ZrO_2 coating

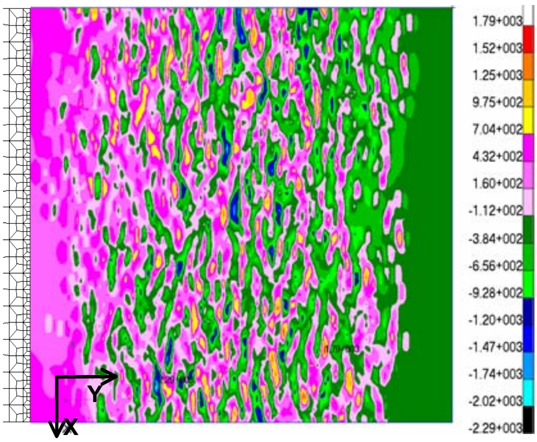

Fig. 3. The plot of residual stress component σ_x

The model mesh in the area of coating is built of square finite elements, which establish a grid of domains in which material properties are randomly defined. Figure 2 presents the model of coating zone with fractions of the materials linearly changing from the pure ZrO_2 ceramics on external surface to the pure steel substrate.

Due to residual stresses distribution assessment the model was thermally and kinematically loaded, adequately by the temperature decrease $\Delta T = -500$ K and the change of the substrate area dimensions.

As the result of calculations the complex distribution of residual stresses was obtained, with the high gradients on the boundary areas between different materials (Fig. 3).

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.

Table 1. Material properties

		beryllium copper substrate	NiCr interlayer	TiN* coating
E	GPa	130	220	600
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, i.e. with or without consideration of microstructure features of the surface coating system.

The set of models, which was used in the study:

Model I – extremely simplified - microstructure features are not taken into considerations,
Model II – transition zones are introduced as graded and they are simulated as multilayered, graded materials,
Model III – transition zones are simulated micromechanically as FGMs,
Model IV – porosity effect in 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 the models I, II and III – properties of the TiN layer are taken like for unporous material (Tab. 1.) and porosity of this layer is simulated micromechanically in the Model IV.

In the Model I (Fig. 4), NiCr as well as TiN volume were treated as homogenous layers, with sharp and straight boundaries between them.

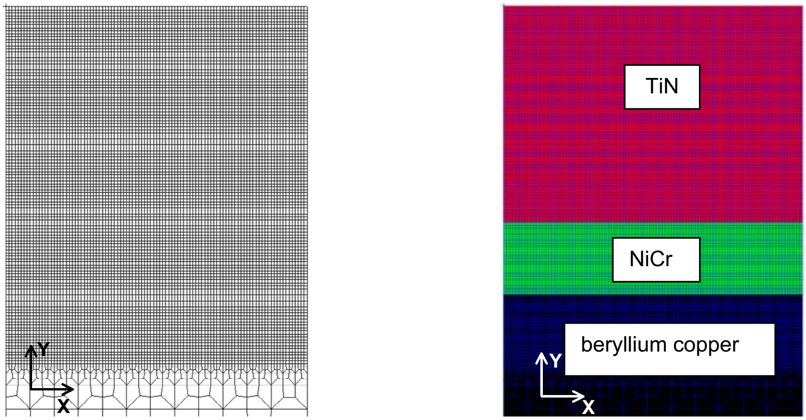

Fig. 4. Model I – a) the area of the surface coating simulation
b) definition of NiCr and TiN layers

Model I doesn't take into consideration such microstructure features like roughness of boundaries between the substrate NiCr and TiN layers, interpenetration of materials of neighboring layers, porosity, voids, micro cracks, etc.

In the Model II (Fig. 5) 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 modeled in such a way may be treated as graded material. Properties of pure materials and volumes of NiCr and TiN were the same like in the Model I. There was assumed that materials in all the layers and introduced sub layers are homogenous. Like the Model I, Model II also doesn't take into consideration such microstructure features like boundaries roughness between the substrate NiCr and TiN layers, interpenetration of materials of neighboring layers, porosity, voids, micro cracks, etc.

In the Model III (Fig.6), transition areas of the same thicknesses were simulated micromechanically as functionally graded materials, with the same linear gradient functions of material properties like in the Model II. In the grid of material domains, material properties were defined in a random way. The linear gradient function of averaged change of material properties in the depth direction was achieved on the way of changing of probability distribution during the drawing of the material in particular domains.

Model III contained the same volumes of materials like Model II and I.

In comparison to these models, it took into consideration interpenetration of materials of neighboring layers, but it still didn't simulate such microstructure features like boundaries roughness between the substrate NiCr and TiN layers, porosity, voids, micro cracks, etc.

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

In the Model IV porosity was introduced into the model with the use of micromechanical approach. Random definition of pores locations that were used in the presented model allowed for the clustering of pores.

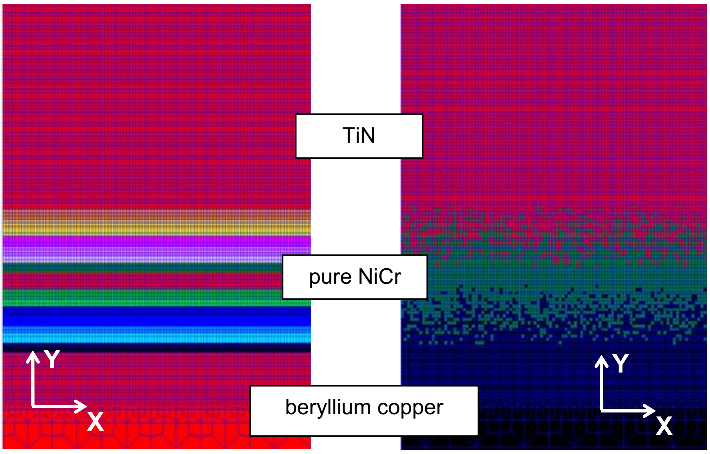

Fig. 5. Model II -transition zones as graded multilayered materials

Fig. 6. Model III - transition zones as functionally graded materials simulated micromechanically

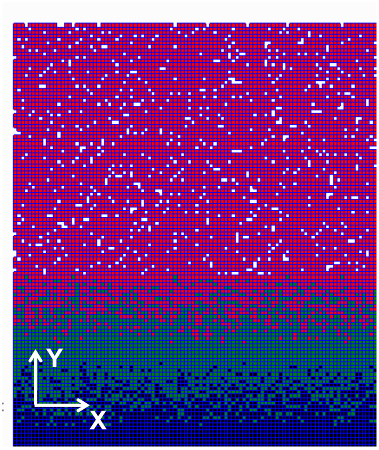

Fig. 7. Model IV - micromechanical simulation of 10% porosity in the TiN layer

4. Results and discussion

Results of residual stresses calculations with the use of the Model I, II and III are adequately presented in the Figures 8÷11.

Model I is the simplest one from the series used for investigations of the TiN surface coating on the beryllium copper substrate, with consideration of the NiCr interlayer.

As the Model I doesn't take into consideration such microstructure features like boundaries roughness between the substrate and NiCr as well as TiN layers, interpenetration of materials of neighboring layers, porosity, voids, micro cracks, etc. – it is not able to produce non zero σ_y residual stress component (in the depth direction).

Strong gradients residual stress component σ_x originates in areas adjacent to boundaries between the NiCr interlayer and the substrate as well as the TiN coating.

Since the thermomechanical properties mismatch between NiCr and unporous TiN is much higher than for NiCr and beryllium copper, the highest gradients of residual stresses were calculated at the boundary between these materials (Fig. 8).

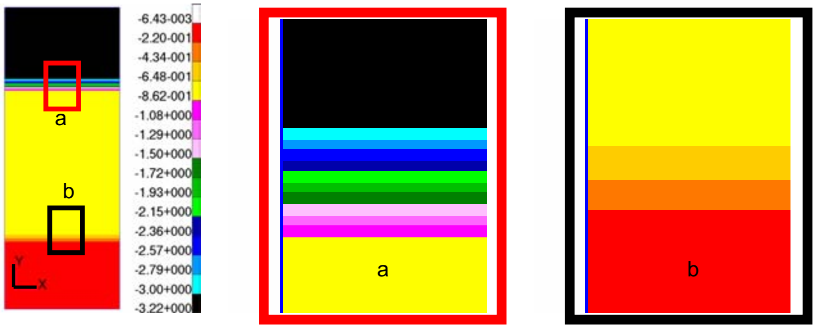

Fig. 8. Model I - the plot of residual stress component σ_x

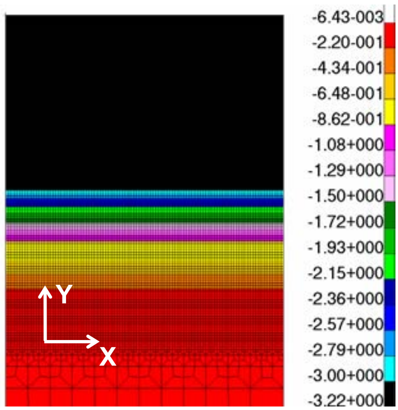

Fig. 9. Model II –the plot of residual stress component σ_x distribution

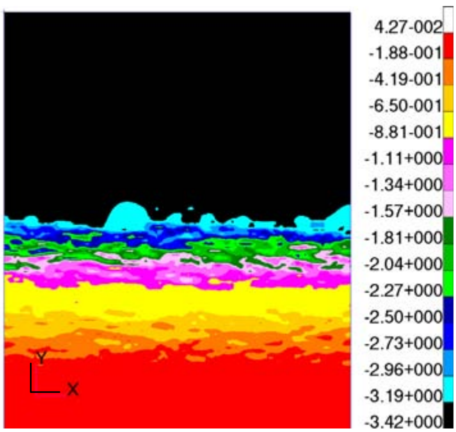

Fig. 10. Model III – the plot of residual stress component σ_x

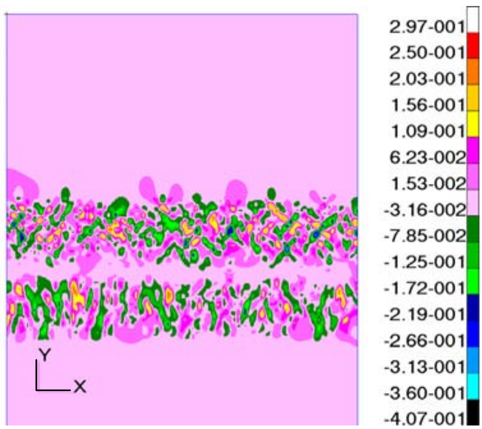

Fig. 11. Model III – the plot of residual stress component σ_y

Model II also 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.

It may be noticed that the range of calculated values of residual stresses are the same in both models: Model II and I. But introducing transition multilayered zones (graded materials) caused redistribution of stresses. As the consequence residual stress gradients were decreased.

Model III, 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. 11). In the areas of homogeneous materials values of the σ_y residual stress component still remain zero.

Another effect of the micromechanically simulated microstructure features is that – in general – values of σ_x component are moved into compression direction (compare Fig. 9 and Fig. 10).

In the transient zone that is modeled micromechanically, interpenetrating material domains act like stress concentrators, causing strong oscillations around the average value counted for the particular depth. Figure 12 presents results for Model II and III 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 modeling of interpenetration of materials in the transient zones, which was performed in Model III shows the microstructural effects.

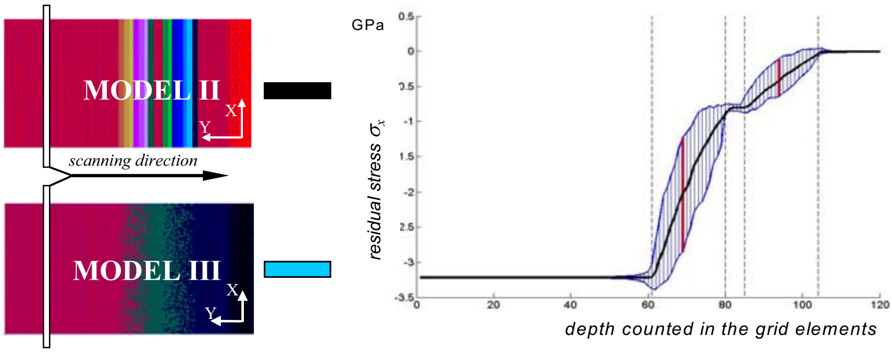

Fig. 12. Comparison of Model II and III – results of scanning in search for extreme values of σ_x stresses in function of the depth (counted in grid element layers, from the free surface of the coating)

Results of calculations for Model IV are presented in figures 13 a, b.

The clustering phenomenon strongly affects these 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 (compare figures 12 and 14).

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.

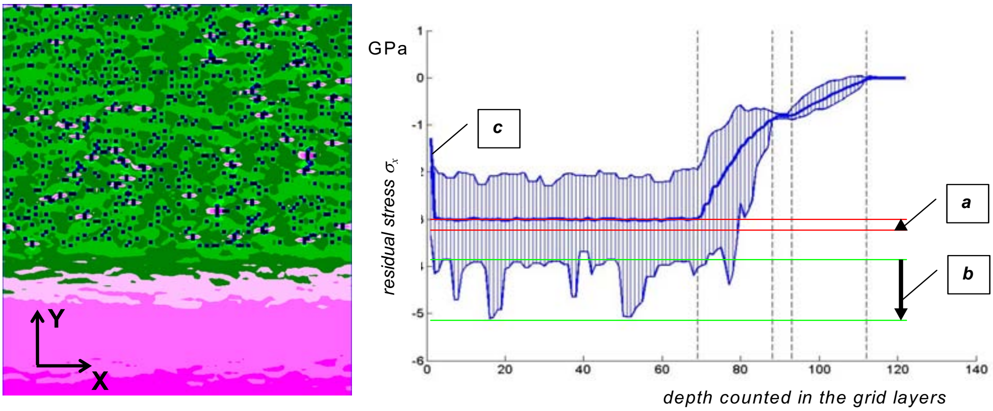

Fig. 13. Model IV - results for the micromechanical simulation of 10% porosity, which allowed for the clustering of pores: a – average value of residual stress σ_x in the TiN layer moves into tensile direction
***b** - the line for the maximum tension shows out the strong effect of the pores clustering*
***c** – the effect of open pores in the free surface*

Simplified models, which may be forced in macro scale by limitations in degrees of freedom avalaible 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.

References

[1] Banks-Skills, L. et al., *Modelling of functionally graded materials in dynamic analyses*, Composites*,* B 33, 7-15, 2002.

[2] Biner, S. B., *Thermo-elastic analysis of functionally graded materials using Voronoi elements*, Mat. Sci. Eng., A315, 136-146, 2001.

[3] Bruck, H. A., *Three-dimensional effects near the interface in a functionally graded Ni-Al_2O_3 plate specimen*, Int. J. Sol. Struct., 39, 547-557, 2002.

[4] Bull, S. J., Bhat, D. G., Staia, M. H., *Properties and performance of commercial TiCN coatings. Part 1: coating architecture and hardness modeling*, Surf. Coat. Techn., 163-164, 499-506, 2003.

[5] Dao, M. et al., *A micromechanical study of residual stresses in functionally graded materials*, Acta Mater., 45(8), 3265-3276, 1997.

[6] Delfosse, D. et al., *Numerical and experimental determination of residual stresses in graded materials*, Composites, Part B, 28B, 127-141, 1997.

[7] Grujicic, M. & Zhao, H., *Optimization of 316 stainless steel/alumina functionally graded material for reduction of damage induced by thermal residual stresses*, Mat. Sci. Eng., A252, 117-132, 1998.
[8] Reiter, T. et al., *Micromechanical models for graded composite materials*, J. Mech. Phys. Solids, 45(8), 1281-1302, 1997.
[9] Shabana, Y.M. & Noda ,N., *Thermo-elasto-plastic stresses in functionally graded materialss subjected to thermal loading taking residual stresses of the fabrication process into considerations*, Composites, Part B 32, 111-121, 2001.
[10] Zuiker, J. R., *Functionally graded materials: choice of micromechanical model and limitations in property variation*, Composites Engineering, 5(7), 807-819, 1995.