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3D-simulation of residual stresses in TBC plasma sprayed coating

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Introduction:

Thermal barrier coatings (TBC) are used in gas turbine technology in order to protect against overheating of the nickel alloy turbine blades. This coating allows to increase turbine inlet temperatures and improve their efficiency(see in (1,2)).

Plasma spraying processes are widely used since several years in thermal barrier coating technology. Although the plasma spraying process of TBC's is largely successful, a fundamental understanding of the processi parameters influencing the TBC microstructure and mechanical properties is necessary. But this investigation has received much less attention so they could lead to considerable advances in performance of plasma sprayed thermal barrier coatings. The main reason of this mate is difficulties in experimental investigation of high temperature and high velocity process . One of the most effective ways to accelerate the process optimization is the application of computer simulation for the modeling of plasma spraying, as shown in (3). This enables the achievement of a maximum of information about the investigated process by carrying out a minimum number of experiments.

The main problem of plasma spray TBC coatings is crack formation during the deposition process and coating cooling. The reasons for this are

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quenched and residual stresses in the coating-substrate system, and peculiarities of TBC coating properties shown in (1-5). The problem of deposition and solidification of plasma sprayed coatings has received little attention to date and remains one of the unintelligible parts of the process. A fundamental understanding of heat transfer in the coating-substrate system and particles deformation processes are, however, critical for the prediction of the microstructural characteristics of the deposited coatings, the understanding of the mechanisms involved in formation of thermal stresses and defects (cracks, debonding etc.).

Residual stress in plasma-sprayed coatings has been recognised as one of their most important properties. It can give rise to deformation of coated workpieces and delamination or cracking of the coating. In addition, various types of coating performance indicators, such as adhesion strength, resistance to thermal shock, life under thermal cycling and erosion resistance are strongly influenced by the nature of the residual stresses (5-8).

Many coating models have been developed. But the majority of them are devoted to mathematical description of macroscopic thermal stresses arising from thermal gradient or mismatches in thermal expansion between the coating and the substrate as it is shown in (5, 8-12). These models usually have a two steps calculation procedure: 1) the solution of the 1D or 2D heat transfer equation with constant boundary conditions using finite difference or finite element methods; 2) computation of thermal residual stresses resulting from temperature history and Hook's law.

The main assumption of this models is the elasticity of the material properties, i.e. the materials behave elastically in the period of heating and cooling, then final residual stress in the coating can simply be expressed as the sum of the stresses arising from differential thermal contraction. But practically, there are a number of stress relaxation processes which may reduce the stress in the splat and coating below its theoretical value (edge relaxation, through-thickness yielding, interfacial sliding, micro- and mackrocracking, creep, delamination etc). The key question concerns the degree to which these relaxation processes can reduce the calculated thermal stresses in practice.

It is necessary to mention, that these relaxation processes are not taken into account in most coating models. This simplification is the basic reason of unconformity of simulation results and experimental measurements of residual stresses.

Stresses can be classified based on the balanced values (I, II and III kind). There are all kinds of stresses presented in plasma spraying coatings,

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but the reasons for crack appearance are stresses of the I kind. Therefore, mostly stresses of this kind are considered in the majority of published experimental and theoretical works. In a first assumption the coating is considered as a continuous medium due to its low porosity. This simplificates sufficiently the problem and allows to carry out calculations in the borders of well designed theories of continuous environment (materials resistance theory, theory of elasticity, plasticity and creep).

For the first time this approach was applied for residual stresses calculation of coatings in work (13) conformably to exploration of thermal stresses in a stripe. Afterwards this method was successfully applied for the determination of thermal residual stresses in coatings of different materials. In work (14) calculations of residual stresses have been done including coating growth and crystallization.

In works (9, 15) the attempt of the account of the residual stresses relaxation is made at the expense of plastic deformation. Therefore, the commercial finite element program ABAQUS is used to calculate residual stresses in the multylayer system. The metallic substrate and the interlayer are calculated according to ideal elastic and ideal plastic material laws. The von Mieses yield condition was used to describe plasticity effects. But, as ceramic coatings have different yield points for compressive and tensile loads, it is difficult to apply the von Misses law to describe plastic deformation in such materials.

A more complete model is offered in (16, 17). The following characteristics serve to define the coating: lamellae structures, quantity of oxide skins, porosity and composition. For lamellae structure formation statistical method and simply Madjesky model, described in (18), were used.

This approach promises a better understanding of mechanical and chemical processes of plasma spraying. But the applied simplified stress-model (elastic) does not give real information about residual stresses, relaxation processes, microcracks formation.

On the base of the above analysis of already developed models it is possible to make the following conclusions:

1) The main assumption of the developed models is elasticity of materials properties, i.e. the materials behave elastically in the period of heating and cooling, final residual stress in the coating is expressed as the sum of the stresses and arises from differential thermal contraction.

2) The stress relaxation processes to caused by macro- and microcrack formation and creep are not taken into account in the most of the developed coating models. This simplification of models is the main reason for the

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inconsistence between modelling results and experimental measurements of residual stresses.

3) The finite element method is suitable and widely used for numerical description of thermophysical and mechanical processes that occur during plasma spray coating formation.

1. Mathematical model of stress generating in plasma coating and its computer realization characteristics:

This work is devoted to the development of models for the simulation of stress formation in TBC-coating with the possibility to implement them into the FEM-MARC program.

More precise and adequate coating models can be developed with 3D finite element simulation by consideration of all relaxation processes. The most common finite element programs are MARC, NASTRAN, ANSYS (see (19, 20)).

The total statement of the thermoelastisity problem consists, as it is described in (21, 22), of the necessity to find out 16 coordinates functions of x_k and time t: 6 components of the stress tensor σ_{ij}, 6 components of the strain tensor ε_{ij} ,3 components of the displacement tensor u_i and temperature T, satisfying 3 movement conditions

$$\sigma_{ij,j} + F_i = \rho \ddot{u}_i \qquad (1)$$

(F_i – volume forces, ρ - material density, $\rho \ddot{u}_i$ - inertia forces), 6 relations between stresses and strains

$$\sigma_{ij} = 2\mu\varepsilon_{ij} + \left[\lambda\varepsilon_{kk} - (3\lambda + 2\mu)\alpha_T\theta\right]\delta_{ij} \qquad (2)$$

(where λ and μ - Lame coefficients in case of isothermal deformation corresponding to defined temperature $T = T_0$), 6 relations between strains and displacements

$$\varepsilon_{ij} = \varepsilon_{ji} = \frac{1}{2}\left(u_{i,j} + u_{j,i}\right) \qquad (3)$$

balance of energy equation:

$$\frac{\partial(\rho(T)C(T)T)}{\partial t} + Q = div(\lambda(T)gradT) \qquad (4)$$

(where $\rho(T)$ – density, C(T) – material heat capacity, Q – internal heat sources/drains density) with fixed boundary and initial conditions.

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Initial conditions are usually given as distributions of displacement vector components u_i, velocities $\dot{u}_i$ and temperatures T in the whole region V of the elastic body. Boundary conditions (BC) on the elastic body surface Σ consists of mechanical and thermal conditions. Mechanical BCs, similar to elasticity theory, are given either in displacements or in stresses. Thermal BCs write as

$$\lambda(T)\frac{\partial T}{\partial n} = Q \tag{5}$$

where $\frac{\partial T}{\partial n}$ - normal derivative, Q – heat flux. In this connection heat flux due to convection and radiation is considered by:

$$q = \sigma\varepsilon(T_s^4 + T_E^4) + \alpha(T_s - T_E) \tag{6}$$

with the emissivity ε of the surface, the heat transfer coefficient α and the Stefan-Boltzmann-number σ=5.669·10^{-8}W/(m^{2}K^4). T_S , T_E and T_G are the temperatures of the surface, environment and plasma-gas.

The set of equations mentioned above describe non-linear thermoelasticity problems even under small strains due to non-linearity of heat transfer equation.

The finite element approximation of equation (4) is based on the Garlerkin version of the method of weighted residuals. As central differential equation for the temperature distribution can be introduced as:

$$\mathrm{C(T)} \cdot \dot{\mathrm{T}} + \mathrm{K(T)} \cdot \mathrm{T} = \mathrm{Q} \tag{7}$$

where $\dot{\mathrm{T}}$ is the nodal temperature vector differentiated with respect to time,

$$\mathrm{C} = \int_{V^e} \rho c \mathrm{N} \cdot \mathrm{N}^{\mathrm{T}} dV^e \tag{8}$$

is the heat capacity matrix, N is the vector of shape functions and K is described as:

$$\mathbf{K} = \int_{V^e} \left(\lambda_x \frac{\partial \mathbf{N}}{\partial x} \cdot \frac{\partial \mathbf{N}^T}{\partial x} + \lambda_y \frac{\partial \mathbf{N}}{\partial y} \cdot \frac{\partial \mathbf{N}^T}{\partial y} + \lambda_z \frac{\partial \mathbf{N}}{\partial z} \cdot \frac{\partial \mathbf{N}^T}{\partial z} \right) dV \tag{9}$$

Q is the nodal heat flux vector due to heat flux through S^e:

$$\mathrm{Q} = \int_{S^e} \mathrm{N} \cdot q dS \tag{10}$$

As ceramic coating have different yield points for compressive and tensile load it is better to use the anisotropic yield function (of Hill) and stress potential are assumed as (19):

$$\sigma = \frac{1}{2}\left[a_1(\sigma_y - \sigma_z)^2 + a_2(\sigma_z - \sigma_x)^2 + \right.$$

$$\left. + a_3(\sigma_x - \sigma_y)^2 + 3a_4\tau_{zx}^2 + 3a_5\tau_{yz}^2 + 3a_6\tau_{xy}^2\right]^{1/2} \quad (11)$$

Ratios of actual to isotropic yield (in the preferred orientation) are defined in MARC for direct tension yielding, and in YRSHR for yield in a shear (the ration of actual shear yield to $\sigma/\sqrt{3}$ isotropic shear yield).

For creep description there are several phenomenological theories. They examine a value v – time derivative of strain or deformation velocity. One of the most frequently used formulas for its calculation is:

$$v(\sigma) = B\sigma^n \quad (12)$$

Numbers n and B are determined experimentally (n is in range of 3 - 8 for various materials). The dependence is strongly nonlinear. The use of exponential dependence is more suitable:

$$\frac{e}{e_e} = \exp\left(\frac{\sigma}{\sigma_e}\right), \quad (13)$$

where e_e and σ_e are properly chosen constants. However, dependence (13) can not be used for small values of σ because it gives non-zero creep velocity when $\sigma = 0$.

The next question concerns the crack appearance and growth. Two problems are solved in crack mechanics. First – prediction of the location of crack initiation and its growth. The second problem stress relaxation due to cracking. Both problems must bee solved together.

Determination of the points where failure can occur in the coating, can be realised using specified failure criteria. In MARC the following criteria are possible: maximum stress (MX STRESS), maximum strain (MX STRAIN), maximum stress for orthotropic materials with identical tensile and compressive behaviour (HILL), Hoffman criterion (HOFFMAN), modified Hill criterion with considering unequal maximum stresses in tension and compression, Tsai-Wu failure criterion - a tensor polynomial criterion-, and user defined failure criteria (subroutine UFAL).

An analysis of these criteria shows, that the Hill criterion is most suitable for plasma coatings. According to this criterion at each integration points, MARC calculates:

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$$\left\{\begin{matrix}\left(\frac{1}{X_t}-\frac{1}{X_c}\right)\sigma_1+\left(\frac{1}{Y_t}-\frac{1}{Y_c}\right)\sigma_2+\frac{\sigma_1^2}{X_tX_c}+ \\ \frac{\sigma_2^2}{Y_tY_c}+\frac{\sigma_{12}^2}{S^2_c}+\frac{\sigma_1\sigma_2}{X_tX_c}\end{matrix}\right\}/F \tag{14}$$

where F- the failure index (normally, F=1.0), X_t , X_c - the maximum allowable stresses in 1-direction in tension and compression, Y_t , Y_c - the maximum allowable stresses in 2-direction in tension and compression, S - the maximum allowable shear stresses.

It permits to determine locations of crack initiation and direction of crack propagation, as crack developed perpendicular to the direction of the maximum principal stress.

For further evaluation of crack propagation nonlinear fracture mechanic models of MARC (J-INTEGRAL, LORENZI) have been used as described in (19).

The extended J-integral takes into account the effect of inertial and body forces, thermal and mechanical loading and initial strains. The expression for the extended J-integral is then transformed into a surface integral for straightforward evaluation of its value, by means of numerical integration techniques.

For plane solid bodies the J-integral can be calculated with the following equation:

$$J=-\int_{\Omega}\frac{1}{\Delta a}\frac{\partial\delta x_l}{\partial\delta x_j}\left(W\delta_{lj}-\sigma_{ij}\frac{\partial u_i}{\partial x_l}\right)dv-$$
$$-\int_{\Omega}\frac{\partial x_l}{\Delta a}\left((f_i-\rho u_i)\frac{\partial u_i}{\partial x_i}-\sigma_{ij}\frac{\partial\varepsilon^0_{ij}}{\partial x_l}\right)dv-\int_{\Gamma_s}\frac{\partial x_l}{\Delta a}t_i\frac{\partial u_i}{\partial x_l}da$$

In this equation regions Ω_1 and Ω_2 have borders Γ_1 and Γ_2 respectively. $\Omega=\Omega_1+\Omega_2$; $\delta x_1=\Delta a$ for border Γ_1 and $\delta x_1=0$ for border Γ_2.

The CRACK DATA option was applied to predict crack initiation and simulate tension softening by plastic yielding and crushing. In this model the cracking option is accessed through the ISOTORPIC option. Normally for this model the following data must be specified: the critical cracking stress, the modulus of the linear strain softening, and the strain at which cracking occurs. It is the critical stress that must be defined at the minimum. It is the stress where cracking occurs in tension. This situation is preferable for plasma spray coating. The crushing strain governs the behaviour in

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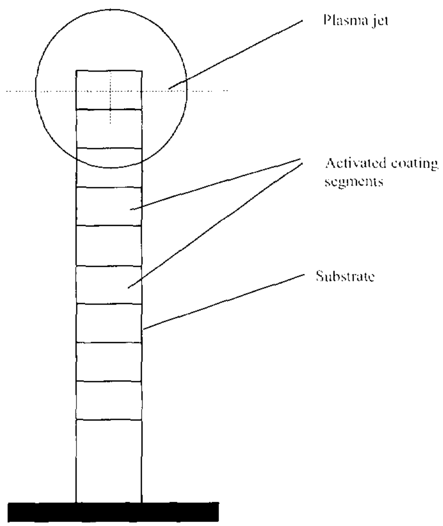
compression. The softening modulus and shear retention factor defines the behaviour after cracking occurs for tension and compression loading, respectively. If tension softening is included, the stress in direction of the maximum stress does not decrease immediately to zero; instead the material softens continously until there is no stress across the crack.

On the base of the above analysis, the development of the following model of stress formation in coating-substrate system under plasma spraying is offered.

The substrate system is represented by a plate (strip) with width 2-3 times smaller than diameter of the plasma jet (120x20x2 mm (Fig.1). A coating with general thickness of 0,06 mm is placed regularly on the whole area of the substrate. The coating is sprayed in one or three passes. The plasma jet moves from the top to the bottom. Coating is ZrO_2 +7%Y_2O_3, substrate is Steel 0,45%C .



a)

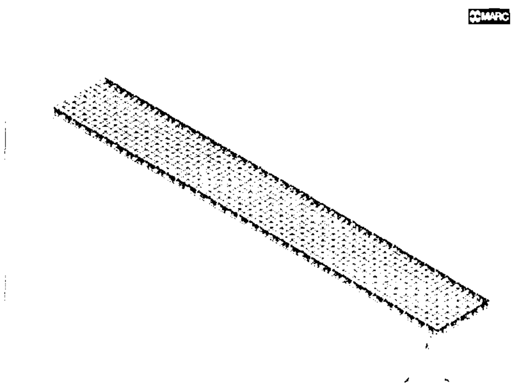

b)

Fig.1. Simulated system, adapted to MARC realisation

The substrate has one fixed edge and the plasma jet moves lengthwise the strip in direction to this edge. The coating is separated along the length into finite segments, which are sequently activated, according to a movement of plasma jet.

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The following stages of plasma spraying process are simulated: 1) consecutive deposition of coating layers with intermediate natural or forced cooling; 2) natural cooling of the coating-substrate system to room temperature. The coating temperature in the moment of deposition is assumed to be melting temperature. Before the beginning of the coating the substrate's temperature is assumed to be 300K.

Ab advantage of such kind of amodel is possibility of its experimental verification with so called „deflection cantilever strip" method discussed in (18).

2. Simulation results and their analysis:

The results of simulation are shown on Figs. 2 – 9.

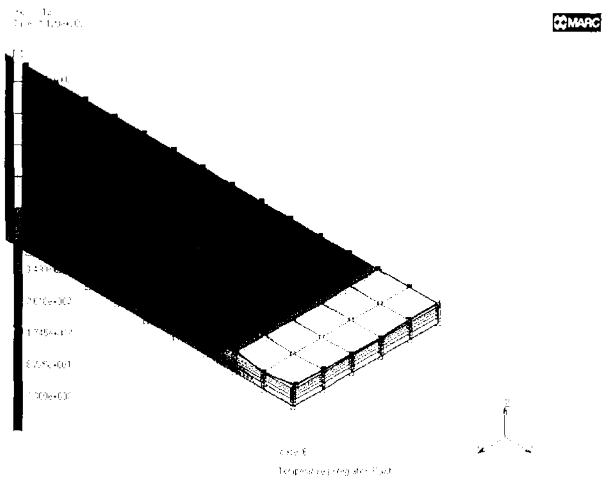

Fig.2. Temperature distribution in a sprayed sample after 7 increments of calculation (activation of 2nd lamella)

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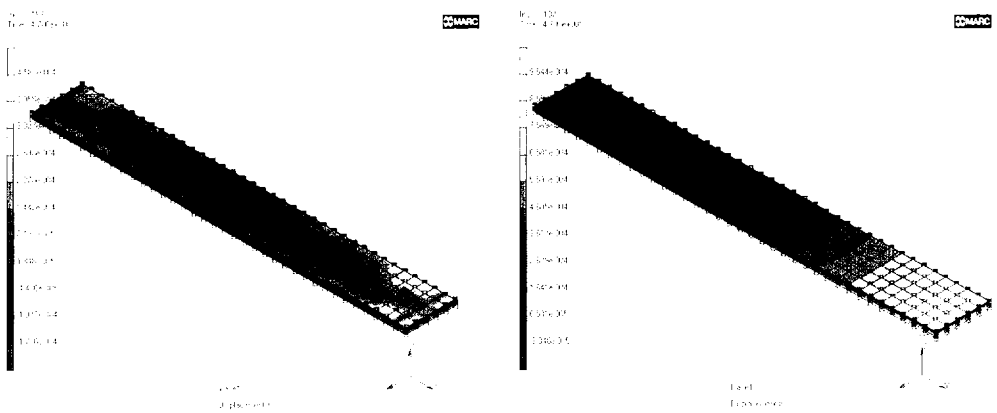
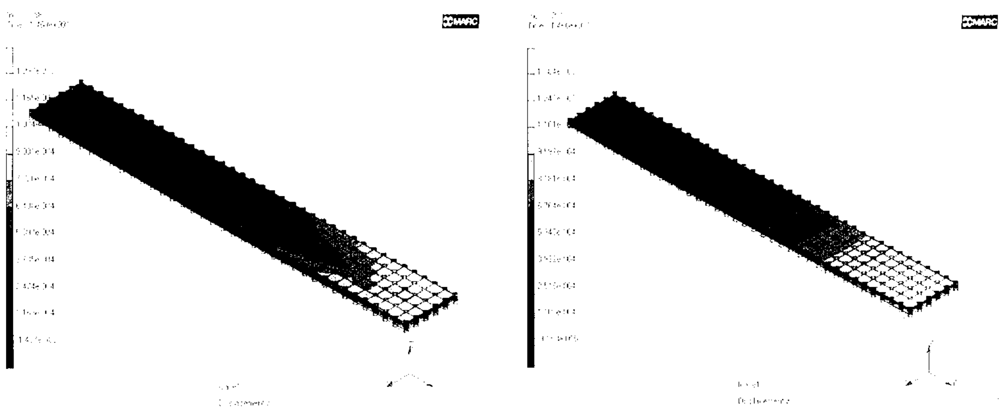


a b

Fig. 3 Displacement of a sprayed sample at the end of spraying – activation of the last of the lamella (a - with cracking, b - without cracking).



a b

Fig. 4. Displacement of a sprayed sample at the end of cooling (a – with cracking, b - without cracking)

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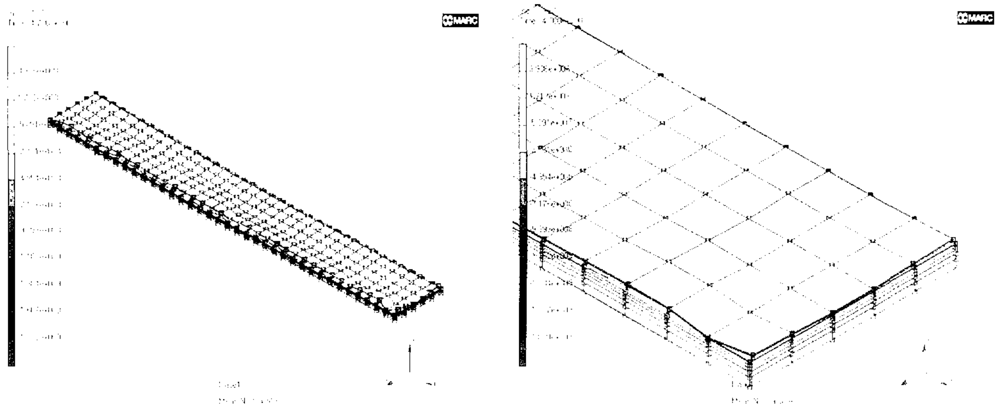
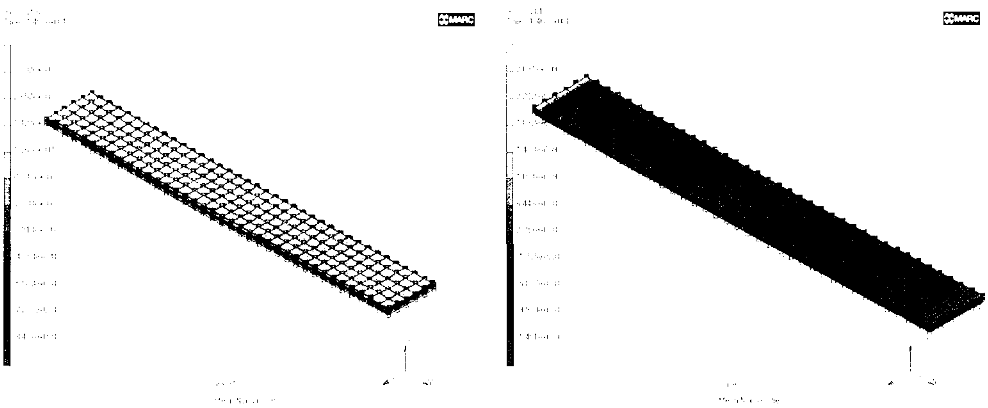


Fig.5. Normal stresses distribution in a sprayed sample after 187 increments (end of spraying – activation of the last lamella) with cracking.



a b

Fig. 6. Normal stresses distribution in a sprayed sample at the end of cooling (a- with cracking, b - without).

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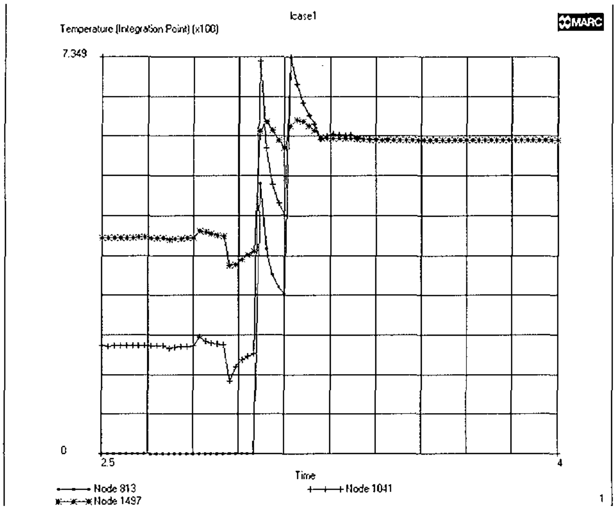

Fig.7. Dynamics of temperature variation on the top of the coating (node 813), in the interface (node 1041) and on the back side of substrate (node 1497)

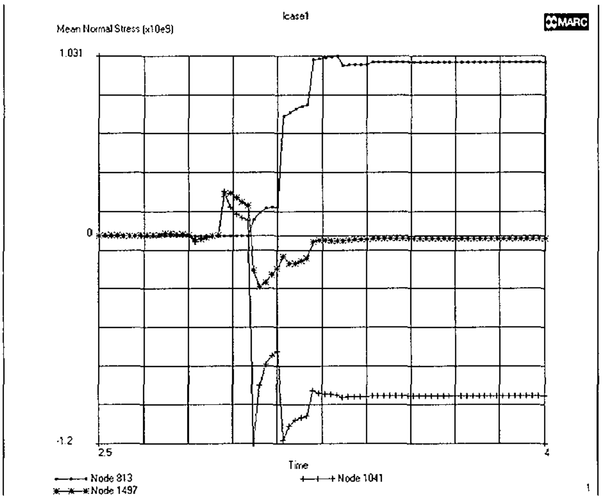

Fig.8. Normal stress dynamics in various points in the thickness of the system (without cracking)

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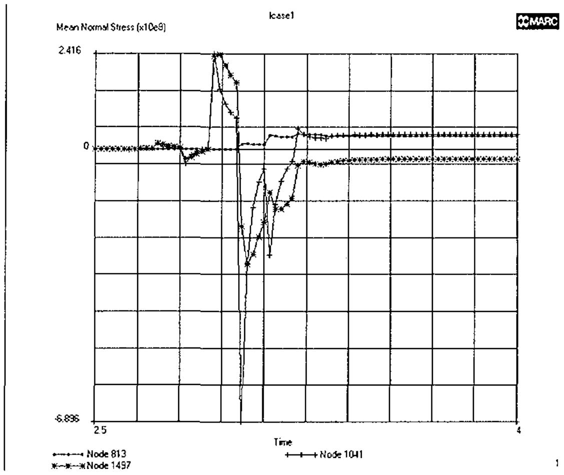

Fig.9.Normal stress dynamics in various points in system height (with cracking)

The analysis of the heating dynamics and the temperature distribution (Figs. 2, 9) shows, that after activating of a lamella the coating temperature rapidly decreases whereas the substrate temperature increases. The maximum temperature gradient is located in the centre of the activated lamella. During spraying the temperature the front moves in the direction of the sample mount. The sprayed parts of the sample at the time of last loadcase activation are cooling down to temperature about 300K.

A general comparison of the sprayed sample displacement in Z-direction (Figs. 3, 4) shows that for the first model (without cracking) the displacement is 10 times higher than for the last model. That can be explained by residual stress relaxation in the last model due to plastic deformation and cracking, because this phenomena are taken into account in the last model. Comparative analysis of normal stress distribution after the end of spraying (Figs.5, 6) verifies this regularity. The level of residual stresses in the elastic model is about 10 times higher than in the cracking model. In the elastic model the bulk of sprayed sample is undergoing tension stresses, in the cracking model – reversed, compression tensions. The obtained results show (Figs. 5, 6, 8, 9), that tension stresses are relaxed due to coating delamination. Delaminations are distributed periodically on the sprayed sample, according to lamella activation.

This regularity can be explained by rapid contraction of an activated coating lamella with generation of tension stresses (maximum in interface)

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due to mismatch in expansion coefficient of coating and substrate materials. But there is a reason for this process in the computation procedure, too. Side by side placing lamellas (with reduced temperature) make hindered contraction in Y-direction for activating and heating lamella. It is one of the reasons for the increase of normal stresses in this place (see Fig. 9, 8) and their relaxation due to cracking and delamination). These reasons for cracking must be eliminated by improvement of model.

3. Conclusions:

1. *Models for heat transfer and stress evaluation during plasma spray* coating for MSC/MARC are developed. These models include the stress relaxation due to plastic deformation, creep and cracking.
2. The first results of simulation are shown:
   - computation of stressess in a coating-substrate system during plasma spraying incorporating stress relaxation due to plastic deformation, creep and cracking give values of sample displacement and stresses about 10 times lower than calculations with an elastic model. This is in accordance with physical phenomena of residual stress formation.
   - the stress relaxation due to cracking is introduced mainly in form of the coating delamination at the place of lamellas activation.
3. One of the ways of model improvment is an the elimination of cracking initiation due to the procedure of coating activation in the calculation procedure.

4. References:

1. T. Troczynsky, S. Cockroft, H. Wong: Key Engineering Materials, Vol. 122-124 (1996), pp. 425-462.
2. W.J. Lackey: Advanced Ceramic Materials 2 (1987), pp.24-32.
3. S. Kundas, A. Dostanko, A. Ilyuschenko at al: “Computer simulation of plasma spraying processes” (Bestprint, Minsk, 1998), pp.10-110 (in Russian)
4. P. Hancock, M. Malik: Materials of Advanced Power Engineering (Kluwer Academic Publishers, London, 1994), pp. 685-704
5. H. Gross, W.Fischer, R.Vasser at al.: Proc. of Int. Conf. "Thermal Spraying' 94",DVS 152. (Essen. Germany - 1994), pp. 260-263.
6. J. Wright, J. Finke, R. Wright at al.: Proceedings of the 8th National Thermal Spray Conference (Houston, Texas, USA, 1995), pp.187-192.

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7. L. Bianchi, P. Lucchesse, A. Denoirjean, P.Fauchais, S.Kuroda : Proceedings of the 8th Thermal Spray Conference, (Houston,USA.-1995), pp. 267-271.
8. C. Funke, B. Siebert, D. Stover, R. Vassen: Proc. of Thermal Spray United Forum for Scienntific and Tegnological Advances (ASM Internnational, Materials Park, Ohio –1998), pp. 227–284.
9. H. Gruhn , W. Mallener, D. Stover: Proceedings of the 8th National thermal Spray Conference (1995,Huston, Texas), pp.231-235.
10. E. Lugsheider, C. Barimani, U. Eritt, Kuzmenkov A.: 15-th Int. Thermal Spray Conference and Exibition (Nice, France, 1998), pp. 367-371.
11. S. Kundas, A. Kuzmenkov, E. Lugsheider, U. Eritt, M. Glißmann: MARC Benutzertreffen (MARC Software GmbH. München, 1998), pp.21-22.
12. H.-D. Steffens, M. Gramlich: Proceedings of the International Thermal Spray Conference & Exposition (Orlando, USA, 1992), pp.531-536.
13. S. Ivanov: Residual stresses , 53(1971), p.84 (in Russian)
14. V. Borvinok: "Control of stress state and properties of plasma coverages" (Moskow, 1990), p.384 (in Russian)
15. H. Gruhn, W. Fischer, C. Funke at al.: Proceedings of the 9th National thermal Spray Conference (1996, Material Park, OH, USA), p.869-874.
16. B. Borgerding: "Zur Simulation von Temperatur- und Spannungsverteilungen in plasmagespritzten Schichtsystemen unter Berücksichtigung der thermophysikalisch relevanten Prozeßdaten" (Mainz. Wiss. Verl. 1994), p.105
17. B. Borgerding, H.J. Solter, E. Lugscheider, K. Simhan: Thermal Spraying.- Vol. 24, N 4(1992), pp. 240-245.
18. Madjesky: Int. J. of Heat and Mass Transfer.- 19(1976),pp
19. MARC Volume A: Theory and user information (MARC Analysis Research Corporation. Palo Alto, CA,USA, 1997) pp.20-150.
20. "MSC/NASTRAN for Windows" pp. 1-300
21. A. Kovalenko: "Thermoelasticity" (Kiev, 1960), pp. 120-130 (in Russian)
22. B. Boli, J. Ueiner: "Thermal stresses theory" (Moscow, High scool, 1960), pp.20-27(in Russian).