

# Numerical solution of the thermomechanical processes in the thin layer structure of thermal barrier<sup>1</sup>

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High demands for dynamic thermal insulating protection of machine parts lead to the development of thermal barriers. The mathematical and simulation model has been developed to simulate thermomechanical processes during thermal shock on the surface of different thermal barrier structures. The finite element method has been applied to the heterogeneous thin layer structure of the thermal barrier. Temperature, temperature gradient, heat flux, thermally induced stress and strain have been chosen as the characteristics describing the dynamic behaviour of the thermal barrier during the thermal shock. Results of the simulation for several alternatives of thermal barrier are discussed to summarize the effect of characteristic parameters of the thermal barrier to its dynamic behaviour.

**Keywords:** computer simulation, FEM, thermomechanical processes, thermal barrier, special industrial application

## 1. INTRODUCTION

Thermal barriers (TB) protect the material of machine parts against high temperatures and thermal shocks. Their importance increases with the orientation to more powerful and economical energy appliances and further in recent advanced manufacturing technologies. TB's usually represent a heterogeneous multilayer coating deposited on the surface of the thermal loaded machine part those temperature should be decreased. Potential advantages of thermal barriers can be summarized into following:

- Keeping the substrate surface temperature of TB-protected machine part at the same value, the appliance operation temperature can be increased along with the increase of the TB thickness that means the higher appliance efficiency.
- On the other hand, using the TB-protected machine part along with keeping the appliance operation temperature at the same value, it leads to the decrease of substrate surface temperature that means the increase of machine part operation lifetime.

The objective of this paper is to shortly point out some specific problems arising from the numerical solution of thermomechanical processes in the TB-substrate system especially during a thermal shock and to show the dynamic behaviour of basic structures of TB in the TB-substrate system. From the physical point of view, it concerns the problem of a non-stationary nonlinear heat and stress distributions in the structured system involving several thin layers of TB and the relatively thick substrate. TB's usually consist of the top ceramic layer, the additional layer and the bond coat. Thermal and mechanical properties of these layers are essentially different. It considerably affects the dynamics of thermal and especially thermal induced stress processes.

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## 2. PHYSICAL STRUCTURE OF THERMAL BARRIERS

The TB structure is given by the technological and operational requirements. The top ceramic layer, usually  $ZrO_2$ , must have high thermal resistivity, sufficient reflectance for infra-red radiation and must satisfy stress and strain conditions. The thickness of the ceramic layer usually ranges from 100 to 500  $\mu m$ . The bond coat must offer fair tolerance against high temperature corrosion and oxidation. Further, the bond coat helps binding the ceramic layer to the substrate and helps accommodating the mechanical deformation caused by different coefficients of thermal expansion and modulus of elasticity for the ceramic layer and the substrate. The bond coat thickness ranges from 100 to 300  $\mu m$ . The additional layer, made of  $Al_2O_3$ , has usually the thickness roughly from 1 to 5  $\mu m$ . This layer represents the diffusion barrier that decreases an oxidation of the bond coat and the underlying substrate.

The thermal conductivity of the ceramic layer is usually about one order lower than of the substrate representing high thermal resistance on the surface. The high thermal resistance decreases the effect of high temperatures and temperature shocks on the surface. The effects of thickness, porosity and thermomechanical properties of each layer to the dynamic behaviour of the TB are the important questions to be solved during the design of TB's. The dynamic behaviour is characterized by the temperature, temperature gradient, heat flux, thermally induced stress and strain, especially at the interface between the individual layers.

The detailed information about the TB physical structure, production, test performance, lifetime modelling, etc., can be found in a relatively numerous literature, particularly in [1, 3, 4, 7, 11, 14, 15, 16, 18].

## 3. MATHEMATICAL MODEL

The machine parts of high temperature appliances are subjected during the operation conditions to various modes of damage including the difference between the thermal expansion coefficients of the ceramic layer and the substrate, phase transformations within the  $ZrO_2$ , erosion, oxidation and high temperature corrosion by molten salts. TB's should be tolerant to these failure modes and should stay well bonded to the substrate during the requested lifetime.

It is impossible to include all of these complicated processes to the computer simulation. The reaction of the TB-substrate structure only at the beginning short time period after the thermal shock on the TB surface is investigated here. Therefore, the processes that are important during long term cyclic thermal loading such as phase transformation within  $ZrO_2$ , oxidation, high temperature corrosion by molten salts, etc. are not taken into account. Only the thermomechanical process of heat transfer and thermally induced stress and strain with the consideration of the elastic mechanical properties is simulated within the TB-substrate structure.

Thermomechanical process in the structure of the TB represents a conjugate process comprising heat transfer and thermally induced stress and strain. Perfect contact between individual layers of a TB and substrate is supposed.

Non-stationary nonlinear heat conduction in individual layers of the TB and the substrate is given by the equation

$$\frac{\partial T}{\partial t} = \frac{1}{C(T)} \frac{\partial}{\partial x_i} \left( \lambda(T) \frac{\partial T}{\partial x_i} \right) + \frac{q_v}{C(T)} \quad (1)$$

where  $C(T) = c(T)\rho(T)$ ,  $c(T)$ ,  $\rho(T)$ ,  $\lambda(T)$ ,  $q_v$ ,  $T$ ,  $t$  and  $x_i$  are temperature dependent volume thermal capacity [ $J \cdot m^{-3} \cdot K^{-1}$ ], temperature dependent specific thermal capacity [ $J \cdot kg^{-1} \cdot K^{-1}$ ], temperature dependent density, temperature dependent coefficient of thermal conductivity, inner heat source, temperature, time and space variables, respectively.

Temperature distribution in the TB induces thermal stress and strain. In the case of a three-dimensional thermally induced stress, six relations between stresses and strains, six relations between

displacements and strains and three equations of continuum equilibrium are to be solved. Fifteen unknown quantities are determined from these relations. These quantities contain six components of the stress tensor  $\sigma_{ij}$ , six components of the strain tensor  $e_{ij}$  and three components of the displacement vector  $u_i$ . The thermally induced stress problem is much more easier, if some quantities are equal to zero or negligible arising from geometry or loads. In the case of plane stress in the plane vertical to the  $z$  axis, the following conditions state

$$\sigma_{zz} = \sigma_{zx} = \sigma_{zy} = 0. \quad (2)$$

The relations between strains, displacements and stresses are then

$$e_{xx} = \frac{\partial u_x}{\partial x} = \frac{1}{E(T)}[\sigma_{xx} - \nu(T)\sigma_{yy}] + \alpha(T)T, \quad (3)$$

$$e_{yy} = \frac{\partial u_y}{\partial y} = \frac{1}{E(T)}[\sigma_{yy} - \nu(T)\sigma_{xx}] + \alpha(T)T, \quad (4)$$

$$e_{xy} = \frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} = \frac{1}{G(T)}\sigma_{xy}, \quad (5)$$

where  $E(T)$  is temperature dependent modulus of elasticity,  $\nu(T)$  is temperature dependent Poisson's ratio,  $\alpha(T)$  is temperature dependent coefficient of thermal expansion and  $G(T)$  is temperature dependent shear modulus

$$G(T) = \frac{E(T)}{2(1 + \nu(T))}.$$

The equilibrium equations are

$$\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{yx}}{\partial y} + f_x = 0, \quad (6)$$

$$\frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} + f_y = 0, \quad (7)$$

where  $f_i$  is the volume strength vector.

The above equations (1)–(7) are supplemented with thermal boundary conditions of the first kind (surface temperature), of the second kind (surface heat flux) and with the boundary surface displacement

$$T(s, t) = F(s, t), \quad Q(s, t) = -\lambda(T) \frac{\partial T(s, t)}{\partial n}, \quad (8)$$

$$u_i(s, t) = L_i(s, t), \quad (9)$$

where  $F(s, t)$ ,  $Q(s, t)$  and  $L_i(s, t)$  are prescribed functions at all surface points  $s$  and time  $t$ ,  $n$  is the outer normal to the surface at the point  $s$ .

Initial conditions are

$$T(x, t) = V(x), \quad \sigma_{ij}(x, t) = W_{ij}(x), \quad (10)$$

where  $V(x)$  and  $W_{ij}(x)$  are prescribed functions at all inner points  $x$ .

Equations (1)–(10) represent the differential mathematical model of the temperature and thermally induced stress processes in the TB-substrate system. Detailed information about mathematical description of the temperature and thermally induced stress fields can be found in [5].

The FEM model of the thermal problem can be written in the following matrix form

$$[C]\{\dot{T}\} + [L]\{T\} = \{q\} \quad (11)$$

where  $[C]$  is the matrix of thermal capacity,  $[L]$  is the matrix of thermal conductivity,  $\{q\}$  is the vector of thermal load and  $\{T\}$ ,  $\{\dot{T}\}$  are the vectors of temperature and temperature time derivative.

Solving this equation for temperature, the thermally induced stress problem can proceed. The matrix form is

$$\{e\} = [B]\{u\} \quad (12)$$

$$\{\sigma\} = [D](\{e\} - \{e_0\}) \quad (13)$$

where  $\{e_0\}$  represents the vector of thermal strain

$$\{e_0\} = \{\alpha\}T, \quad (14)$$

$\{e\}$ ,  $\{\sigma\}$  and  $\{u\}$  are the vectors of strain, stress and nodal displacements.  $[B]$  is the strain-displacement matrix,  $[D]$  is the elasticity matrix and  $\{\alpha\}$  is the vector of linear thermal expansion.

Combining the equilibrium conditions (6), (7) with boundary conditions (8), (9) leads to the matrix equation

$$[K]\{u\} = \{f\} \quad (15)$$

where

$$[K] = [B]^T[D][B], \quad (16)$$

$$\{f\} = [B]^T\{\sigma\}. \quad (17)$$

$[K]$  is the standard stiffness matrix and  $\{f\}$  is the vector of nodal forces corresponding to the boundary conditions. Further information about FEM modelling of thermal stress problems can be found in [19].

#### 4. PHYSICAL PROPERTIES OF TB MATERIALS

The TB-substrate structure represents a nonlinear heterogeneous thermomechanical system. It is important to get the sufficiently accurate thermal and mechanical properties of individual TB and substrate materials. Inaccuracy of these material parameters significantly affects the results of a numerical solution, particularly when the dynamic TB behaviour is analyzed.

Following these arguments the detailed analysis of thermal and mechanical properties have been made. The available published experimental data have been collected and analytical temperature dependence of the individual material properties has been proposed.

Thermal conductivity  $\lambda$ , specific thermal capacity  $c$  and density  $\rho$  belong to the most important thermal parameters, whereas modulus of elasticity  $E$ , thermal expansion  $\alpha$  and Poisson's ratio  $\nu$  are the most important mechanical parameters. The following analytical functions of temperature are valid at least for  $T \in (273, 1273 \text{ K})$ .

##### 4.1. Material properties of $\text{ZrO}_2$

Zirconia oxide is a ceramic material whose thermal and mechanical properties varies significantly with porosity  $p$  [-].

Porosity dependence of thermal conductivity  $\lambda$  [ $\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ ] is given by

$$\begin{aligned} \lambda &= 3.230 \times 10^{-4}T + 1.782 & p < 0-3\% \\ \lambda &= 3.840 \times 10^{-4}T + 1.475 & p < 3-10\% \\ \lambda &= 5.040 \times 10^{-4}T + 1.252 & p < 10-16\% \\ \lambda &= 2.530 \times 10^{-7}T^2 + 1.086 \times 10^{-5}T + 9.442 \times 10^{-1} & p < 16-20\% \\ \lambda &= 2.360 \times 10^{-7}T^2 + 1.014 \times 10^{-5}T + 8.826 \times 10^{-1} & p < 20-24\% \\ \lambda &= -1.825 \times 10^{-13}T^4 + 6.361 \times 10^{-10}T^3 \\ &\quad - 3.818 \times 10^{-7}T^2 + 7.608 \times 10^{-5}T + 5.637 \times 10^{-1} & p < 24-30\% \end{aligned}$$

Porosity dependence of density  $\rho$  [ $\text{kg}\cdot\text{m}^{-3}$ ] is given by

$$\begin{array}{ll} \rho = 5950 & p \langle 0-3\% \rangle \\ \rho = 5645 & p \langle 3-10\% \rangle \\ \rho = 5245 & p \langle 10-16\% \rangle \end{array} \quad \begin{array}{ll} \rho = 4940 & p \langle 16-20\% \rangle \\ \rho = 4695 & p \langle 20-24\% \rangle \\ \rho = 4395 & p \langle 24-30\% \rangle \end{array}$$

Other thermal and mechanical material properties of the material are given as

$$\begin{array}{ll} c = 6.110 \times 10^{-2}T + 5.650 \times 10^2 - 1.141 \times 10^7T^{-2} & [\text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}] \\ \alpha = -2.482 \times 10^{-12}T^2 + 7.568 \times 10^{-9}T + 4.037 \times 10^{-6} & [\text{K}^{-1}] \\ E = -5.367 \times 10^7T + 1.844 \times 10^{11} & [\text{Pa}] \\ \nu = 0.290 & [-] \end{array}$$

#### 4.2. Material properties of Nimonic 90

This alloy represents bond coat between ceramic layer and substrate. Chemical composition of Nimonic 90 is 58% Ni – 20% Cr – 18% Co – 3% Ti – 1% Al. Temperature dependence of thermal and mechanical properties is given by

$$\begin{array}{ll} \lambda = 2.277 \times 10^{-6}T^2 + 1.472 \times 10^{-2}T + 7.198 & [\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}] \\ c = 2.130 \times 10^{-8}T^2 + 5.738 \times 10^{-1}T + 8.155 \times 10^1 & [\text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}] \\ \rho = -1.397 \times 10^{-4}T^2 - 1.900 \times 10^{-1}T + 8.336 \times 10^3 & [\text{kg}\cdot\text{m}^{-3}] \\ \alpha = 3.734 \times 10^{-12}T^2 + 4.109 \times 10^{-10}T + 1.124 \times 10^{-5} & [\text{K}^{-1}] \\ E = -8.103 \times 10^1T^3 + 2.046 \times 10^4T^2 + 1.346 \times 10^7T + 2.129 \times 10^{11} & [\text{Pa}] \\ \nu = 1.509 \times 10^{-8}T^2 + 1.161 \times 10^{-5}T + 3.136 \times 10^{-1} & [-] \end{array}$$

#### 4.3. Material properties of steel ČSN 17246

Refractory steel ČSN 17246 represents substrate. Chemical composition of this steel is Fe – 17.0–20.0% Cr – 8.0–11.0% Ni – max. 2.0% Mn – max. 1.0% Si – max. 0.12% C – max. 0.045% P – max. 0.030% S. Temperature dependence of thermal and mechanical properties is given by

$$\begin{array}{ll} \lambda = 3.959 \times 10^{-6}T^2 + 9.015 \times 10^{-3}T + 1.292 \times 10^1 & [\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}] \\ c = -1.144 \times 10^{-4}T^2 + 3.102 \times 10^{-1}T + 3.934 \times 10^2 & [\text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}] \\ \rho = -2.505 \times 10^{-5}T^2 - 0.400T + 8.016 \times 10^3 & [\text{kg}\cdot\text{m}^{-3}] \\ E = 2.331 \times 10^4T^2 - 1.013 \times 10^8T + 2.238 \times 10^{11} & [\text{Pa}] \\ \alpha = -1.204 \times 10^{-12}T^2 + 5.723 \times 10^{-9}T + 1.457 \times 10^{-5} & [\text{K}^{-1}] \\ \nu = 5.852 \times 10^{-8}T^2 - 2.456 \times 10^{-5}T + 2.951 \times 10^{-1} & [-] \end{array}$$

The tabular data for the TB individual layers and the substrate used to create the above relations are taken mainly from [2, 6, 12, 13, 17].

Table 1. Values of material properties at temperature 673 K

material property	unit	ZrO <sub>2</sub>	Nimonic 90	ČSN 17246
thermal conductivity $\lambda$	$[\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}]$	1.066	18.14	20.78
specific thermal capacity $c$	$[\text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}]$	580.9	467.7	550.3
density $\rho$	$[\text{kg}\cdot\text{m}^{-3}]$	4940	8145	7735
modulus of elasticity $E$	$[\text{GPa}]$	148.3	206.5	166.2
thermal expansion $\alpha$	$10^6 [\text{K}^{-1}]$	8.010	13.21	17.90
Poisson's ratio $\nu$	$[-]$	0.290	0.328	0.305

The values of TB and substrate material properties at temperature 673 K are presented in Table 1 to show the heterogeneous structure of TB and substrate.  $ZrO_2$  of 16–20% porosity is considered there.

## 5. RESULTS

The computational system MARC implements transformation of the problem to the computational model utilizing the finite element method (FEM). MARC capabilities of solving non-linearities caused by the temperature dependent material properties and boundary conditions are utilized in modelling the dynamic behaviour of TB under the thermal shock. One interested in using MARC can see [8, 9, 10].

The planar geometry and boundary conditions are plotted in Fig. 1. Zero stress and the temperature of 293 K in the whole TB-substrate structure have been taken as the initial conditions. Elements of the discretization grid within the TB layers have the thickness  $5 \mu\text{m}$  for the proper resolution of the solved quantities in the individual layers of TB and especially near the interface between adjacent layers. The thickness of elements in the substrate is linearly increasing with the distance from the surface. The time step is set to 1 ms.

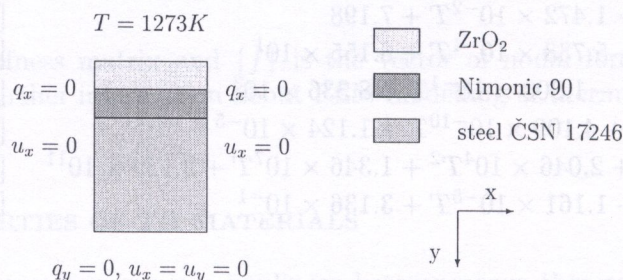

 $x$   
 $y$ 

Fig. 1. Geometry and boundary conditions of the model

The effect of the time step on the substrate surface temperature at 1 s for the case of one-layer TB ( $ZrO_2$  of 1 mm thickness and 3–10% porosity) can be seen on the values of the dimensionless temperature  $\Theta = T/T_{ref}$ , where  $T_{ref}$  is the temperature for the case of time step 1 ms ( $\Theta = 1.000$  for the time step 1 ms,  $\Theta = 0.999$  for 10 ms,  $\Theta = 0.990$  for 100 ms and  $\Theta = 0.920$  for 1000 ms).

The effect of the thickness of elements of the discretization grid is similar. The dimensionless temperature is given by  $\Theta = T/T_{ref}$ , where  $T_{ref}$  is the temperature for the elements thickness  $5 \mu\text{m}$  in the TB ( $\Theta = 1.000$  for the elements thickness  $5 \mu\text{m}$ ,  $\Theta = 0.997$  for  $20 \mu\text{m}$ ,  $\Theta = 0.989$  for  $67 \mu\text{m}$  and  $\Theta = 0.962$  for  $250 \mu\text{m}$ ).

A number of the various TB-substrate structures have been solved including raw substrate, one-layer and two-layer TB's.

### 5.1. Influence of TB parameters on the substrate surface temperature

In the case of the substrate without a TB, surface temperature is 1273 K. With  $ZrO_2$  of 1 mm thickness and 3–10% porosity, substrate surface temperature decreases to 450 K after 1 s. With the increase of the  $ZrO_2$  thickness to 2 mm, substrate surface temperature decreases to 323 K after 1 s. With  $ZrO_2$  of 1 mm thickness and 16–20% porosity, substrate surface temperature decreases only to 383 K after 1 s. By the presence of  $ZrO_2$  of 1 mm thickness and 3–10% porosity and Nimonic 90 of 1 mm thickness, substrate surface temperature decreases to 393 K after 1 s. The greater Nimonic 90 thickness, the lower substrate surface temperature is reached. Considerable influence of the TB on the substrate surface temperature is evident from the above substrate surface temperature values.

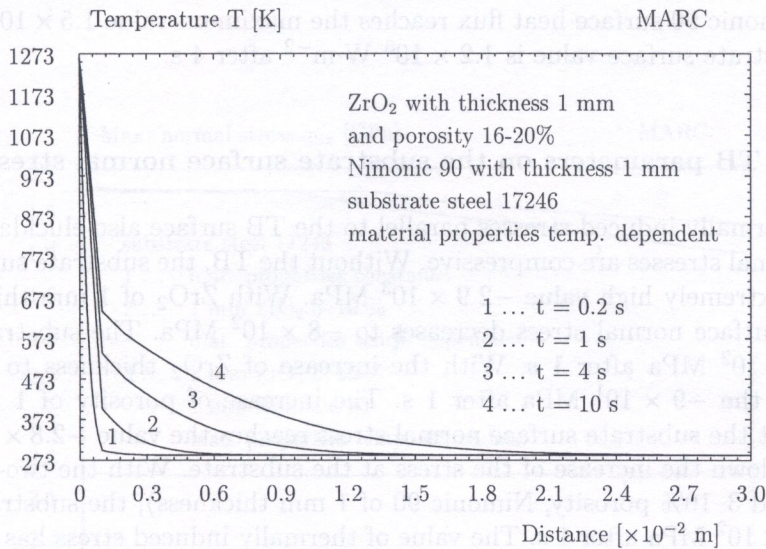


Fig. 2. Temperature dependence on the distance from the surface

The temperature dependence on the distance from the surface at 0.2, 1, 4 and 10 s for the two-layer TB is shown in Fig. 2.

## 5.2. Influence of TB parameters on the substrate surface temperature gradient

In the case of the substrate without a TB, substrate surface temperature gradient reaches the extremely high value of  $-4.1 \times 10^5 \text{ K}\cdot\text{m}^{-1}$  after 0.2 s,  $-1.8 \times 10^5 \text{ K}\cdot\text{m}^{-1}$  after 1 s. With  $\text{ZrO}_2$  of 1 mm thickness and 3–10% porosity, surface temperature gradient at the external surface increases to  $-1.8 \times 10^6$  after 0.2 s, but at the same time substrate surface temperature gradient decreases to  $-3 \times 10^4 \text{ K}\cdot\text{m}^{-1}$ .

The  $\text{ZrO}_2$  surface temperature gradient decreases in time, meanwhile temperature gradient near the  $\text{ZrO}_2$  – underlying material interface increases so that the maximum value of temperature gradient moves from the  $\text{ZrO}_2$  surface to the  $\text{ZrO}_2$  – underlying material interface.

The substrate surface temperature gradient reaches the value  $-7.5 \times 10^4 \text{ K}\cdot\text{m}^{-1}$  after 1 s in the case of 1 mm thick  $\text{ZrO}_2$  and 3–10% porosity. With the increase of  $\text{ZrO}_2$  thickness to 2 mm, substrate surface temperature gradient reaches the value  $-1.1 \times 10^4 \text{ K}\cdot\text{m}^{-1}$  after 1 s. Increasing the  $\text{ZrO}_2$  porosity, substrate surface temperature gradient decreases. The presence of Nimonic 90 causes further decrease of temperature gradient on the substrate surface.

## 5.3. Influence of TB parameters on the substrate surface heat flux

At the open substrate surface, heat flux reaches the value of  $1.3 \times 10^7 \text{ W}\cdot\text{m}^{-2}$  after 0.2 s and after 1 s it decreases to  $5.6 \times 10^6 \text{ W}\cdot\text{m}^{-2}$ .

With  $\text{ZrO}_2$ , maximum heat flux values moves in time from the  $\text{ZrO}_2$  surface to its interface with the underlying material. It is the similar behaviour as is observed for the temperature gradient.

With  $\text{ZrO}_2$  of 1 mm thickness and 3–10% porosity, the maximum value of heat flux at the substrate surface  $1.3 \times 10^6 \text{ W}\cdot\text{m}^{-2}$  is reached after 1 s. Then, the heat flux is slowly decreasing in time. With the increase of  $\text{ZrO}_2$  thickness to 2 mm, substrate surface heat flux has a maximum value  $6.5 \times 10^5 \text{ W}\cdot\text{m}^{-2}$  after 4 s. In the case of  $\text{ZrO}_2$  of 1 mm thickness, increasing the porosity to 16–20%, the substrate surface heat flux reaches the maximum value  $9 \times 10^5 \text{ W}\cdot\text{m}^{-2}$  after 4 s. In the presence of Nimonic 90, heat flux increases in the bond coat area, but decreases at the substrate surface. With two-layer TB ( $\text{ZrO}_2$  of 1 mm thickness and 3–10% porosity, Nimonic 90 of 1 mm

thickness), the Nimonic 90 surface heat flux reaches the maximum value  $1.5 \times 10^6 \text{ W}\cdot\text{m}^{-2}$  after 1 s, the maximum substrate surface value is  $1.2 \times 10^6 \text{ W}\cdot\text{m}^{-2}$  after 4 s.

#### 5.4. Influence of TB parameters on the substrate surface normal stress

The analysis of thermally induced stresses parallel to the TB surface also elucidates the role of TB. All the surface normal stresses are compressive. Without the TB, the substrate surface normal stress reaches constant extremely high value  $-2.9 \times 10^3 \text{ MPa}$ . With  $\text{ZrO}_2$  of 1 mm thickness and 3–10% porosity, the TB surface normal stress decreases to  $-8 \times 10^2 \text{ MPa}$ . The substrate surface normal stress gets  $-4.7 \times 10^2 \text{ MPa}$  after 1 s. With the increase of  $\text{ZrO}_2$  thickness to 2 mm, its surface value decreases to the  $-9 \times 10^1 \text{ MPa}$  after 1 s. The increase of porosity of 1 mm  $\text{ZrO}_2$  layer to 16–20% causes that the substrate surface normal stress reaches the value  $-2.8 \times 10^2 \text{ MPa}$  after 1 s. Nimonic 90 slows down the increase of the stress at the substrate. With the two-layer TB ( $\text{ZrO}_2$  of 1 mm thickness and 3–10% porosity, Nimonic 90 of 1 mm thickness), the substrate surface normal stress reaches  $-3 \times 10^2 \text{ MPa}$  after 1 s. The value of thermally induced stress has overcome stability limit of used materials because of only thermoelastic problem has been solved.

The changes of the normal stress  $\sigma_{xx}$  along the distance from the surface of the two-layer TB are shown in Fig. 3. One can clearly observe how the Nimonic 90 surface and the substrate surface compressive stresses increase as they overcome the TB surface stress.

The influence of the TB structure on time changes of the maximum stresses in the TB and substrate is shown in Fig. 4. The TB surface normal stresses are nearly time independent, except for the beginning of the thermal shock. Constant values of normal stress indicate that neither Nimonic 90 nor substrate surface values do overcome the TB surface value. With Nimonic 90, the increase of maximum value of normal stress within the Nimonic 90 and substrate is slowed and moved to longer times. Nimonic 90 surface stress overcomes the TB surface stress at approximately 4.2 s, substrate surface stress overcomes the TB and Nimonic 90 surface stresses somewhere between 4 and 10 s. The increase of substrate normal stress is considerably slower than in the TB without Nimonic 90.

Figure 5 shows the influence of  $\text{ZrO}_2$  thicknesses on the maximum stresses in the structure  $\text{ZrO}_2$ -substrate. For the TB of 0.5 mm thick  $\text{ZrO}_2$ , the substrate surface normal stress exceeds the TB surface value at 0.8 s. With the increase of  $\text{ZrO}_2$  thickness to 1 mm, this time point moves to 3 s. The increase of  $\text{ZrO}_2$  thickness to 2 or 4 mm moves this time point behind the 10 s.

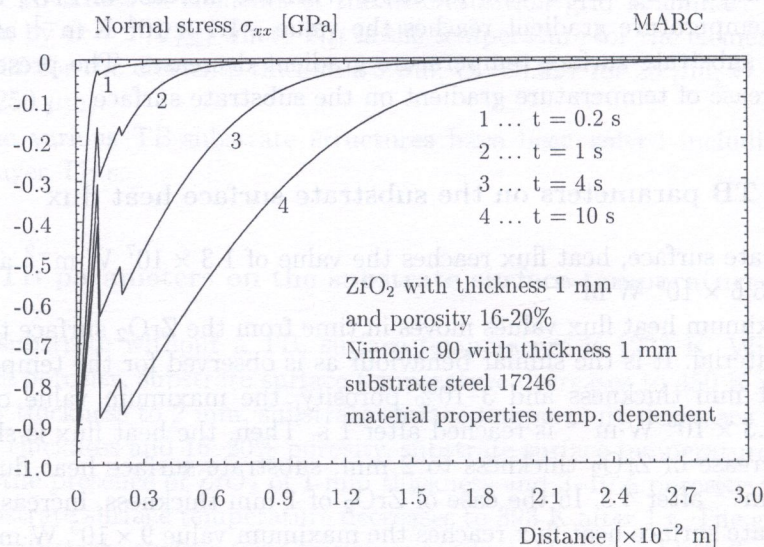


Fig. 3. Normal stress dependence on the distance from the surface



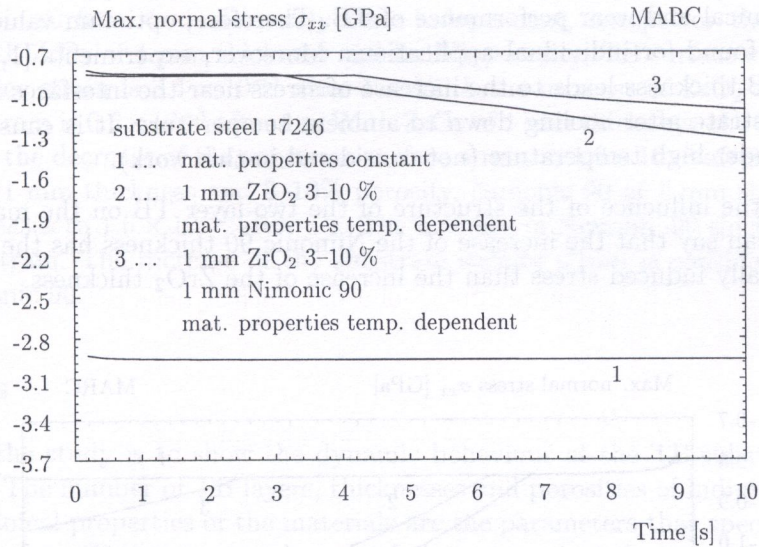


Fig. 4. Maximum normal stress time dependence – TB's usage

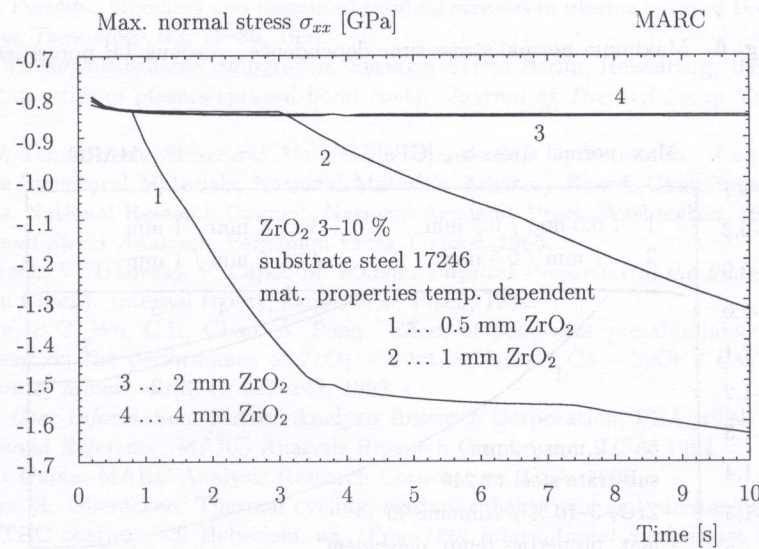


Fig. 5. Maximum normal stress time dependence – various TB thicknesses

Figure 6 shows the influence of ZrO<sub>2</sub> porosities on the maximum stresses in the structure ZrO<sub>2</sub>-substrate. With the increase of ZrO<sub>2</sub> porosity, the increase of the substrate surface stress is slowed. We can say that the higher thickness and porosity of ZrO<sub>2</sub>, the lower stresses will be thermally induced. However, increasing the thickness and porosity of ZrO<sub>2</sub> has the opposite effect – the decrease of mechanical, chemical and wear performance of TB. Therefore, optimum values of thickness and porosity has to be found for individual applications. Moreover, experiments [1, 11] show that the large increase of TB thickness leads to the increase of stress near the interfaces between individual TB layers and substrate after cooling down to ambient temperature. It is caused by the effect of stress relaxation under high temperature (not considered in this work).

Figure 7 shows the influence of the structure of the two-layer TB on the maximum stresses in the structure. We can say that the increase of the Nimonic 90 thickness has the significantly lower effect on the thermally induced stress than the increase of the ZrO<sub>2</sub> thickness.

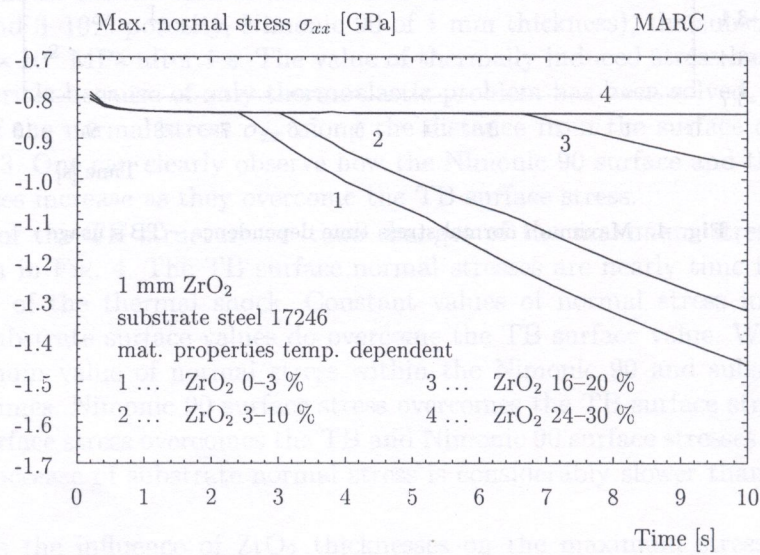


Fig. 6. Maximum normal stress time dependence – various TB porosities

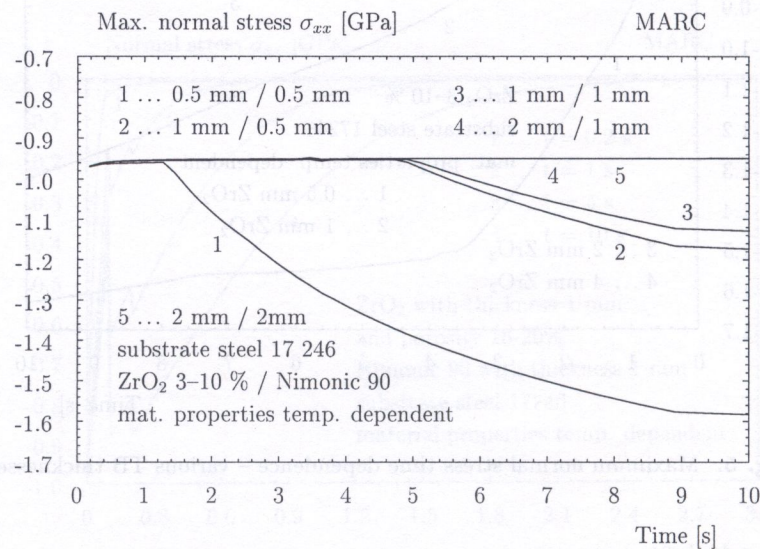


Fig. 7. Maximum normal stress time dependence – two-layer TB's

### 5.5. Influence of TB parameters on the substrate surface strain

Differences in thermally induced strains of each individual TB layer and of the substrate often lead to the spallation of TB. In the case of the substrate without TB, the substrate surface strain is  $2.29 \times 10^{-2}$ . This surface strain is nearly time independent, except for the beginning of the thermal shock. With ZrO<sub>2</sub> of 1 mm thickness and 3–10% porosity, TB surface strain is  $8.8 \times 10^{-3}$ , but substrate surface strain is  $3.4 \times 10^{-3}$  after 1 s. With the increase of ZrO<sub>2</sub> thickness to 2 mm, substrate surface strain is  $0.6 \times 10^{-3}$  after 1 s. With ZrO<sub>2</sub> of 1 mm thickness, the increase of porosity to 16–20% leads to the decrease of the substrate surface strain to  $1.9 \times 10^{-3}$  after 1 s. With the two-layer TB (ZrO<sub>2</sub> of 1 mm thickness and 3–10% porosity, Nimonic 90 of 1 mm thickness), substrate surface strain decreases to  $1.6 \times 10^{-3}$  after 1 s. The increase of Nimonic 90 thickness decreases the substrate surface strain. The increase of the substrate surface strain is considerably slowed down by the use of Nimonic 90.

### 6. CONCLUSIONS

The main task of the study is to show the dynamic behaviour of the TB-substrate system under the thermal shock. The number of TB layers, thicknesses and porosities of individual TB layers and thermal and mechanical properties of the materials are the parameters that specify the structure of the TB-substrate system. The structure subsequently influences the behaviour of this system. Special attention has to be paid to get the accurate thermal and mechanical properties of the materials. The presented results confirm the importance of TB's as a dynamic material protection against the thermal overloading. The stress relaxation under high temperature appears as an additional significant process that has not been considered yet. Therefore, the effect of stress relaxation along with the effect of residual stresses after the TB deposition is prepared to be encountered to the future modelling of TB behaviour under the condition of thermal shock.

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CONCLUSIONS

The main task of the study is to show the dynamic behaviour of the TBC-substrate system under the thermal shock. The number of TBC layers, thickness and porosity of individual TBC layers and thermal and mechanical properties of the materials are the parameters that affect the structure of the TBC-substrate system. The structure significantly influences the behaviour of this system. Special attention has to be paid to get the accurate thermal and mechanical properties of the materials. The present results confirm the importance of TBC as a dynamic thermal protection against the thermal overloading. The stress relaxation under high temperature appears as an additional significant process that has not been considered yet. Therefore, the effect of stress relaxation along with the effect of residual stresses after the TBC deposition is required to be accounted in the future modelling of TBC behaviour under the condition of thermal shock.

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