Simulation of thermal barrier coating behaviour during dynamic thermal loading by the Exodus method

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Abstract

This paper deals with the application of the stochastic Exodus method in simulation of the heat transfer processes in the multi-layer structure of thermal barrier coating. A 2D computer simulation model of thermal barrier behaviour during its dynamic thermal loading is presented. The Exodus stochastic simulation method has been applied to solve the indirect thermal problem in order to determine TBC surface temperature and heat flux from the temperatures measured inside the sample. Comparison of the computer results with the result of the thermography measurement is presented to show capabilities of the simulation model.
Keywords: Exodus simulation method, computer modelling, thermal barrier coatings, thermography measurement.

1 Introduction

Thermal barriers protect material of machine parts against high temperatures and thermal shocks. Thermal barriers usually represent a heterogeneous multilayer coating deposited on the surface of thermally loaded machine parts those temperature should be decreased.

The Exodus method [1], which is a modification of the Monte Carlo method [2], has been used, in order to determine the transient state distribution of barrier dynamic behaviour during thermal shocks in this paper. From the physical point of view, it concerns the problem of a non-stationary heat distribution in a structured system involving several thin layers of thermal barrier [3] and

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substrate. Thermal barrier usually consists of the top ceramic layer, the additional layer and the bond coat. Thermal properties of these layers are essentially different.

Dynamical loadings of TBCs [4] by a thermal spray gun hot exhaust gases to simulate periodic short-term thermal shocks belong to TBC performance tests. Temperature inside the sample is measured by thermocouples, surface temperature distribution is measured by IR thermography.

The problem of heat transfer in the thin layer structure of thermal barrier has been solved by means of various methods [5, 6]. So far, no attention has been paid to the practical possibilities of solving the problem by the application of probabilistic methods. Nevertheless the stochastic methods have some advantages in determination of surface temperatures and heat fluxes as a measure of TBC quality. As direct measurement of surface temperature and heat flux during the TBC tests is difficult, an indirect thermal problem is solved based on the temperatures measured inside the sample volume.

2 Thermal barriers and their tests

2.1 Thermal barrier coatings

The thermal barrier structure [6] is given by the technological and operational requirements. The top ceramic layer, usually ZrO_2, must have high thermal resistivity, sufficient reflectance for infrared radiation and must satisfy stress and strain conditions. The thickness of the ceramic layer usually ranges from 100 to 500 μm. 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 μm. The additional layer, made of Al_2O_3, has usually the thickness roughly from 1 to 5 μm. This layer represents a diffusion barrier that decreases oxidation of the bond coat and the underlaying 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 temperatures shocks on the surface. The effect of thickness, porosity and thermomechanical properties of each layer to the dynamic behaviour of the thermal barrier are the important questions to be solved during the TBC design. 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.

2.2 TBC dynamic tests and measurement

The thermal barrier sample has been thermally loaded by cyclic passing of torch over the surface (fig. 1). Torch-sample distance 120 mm and torch velocity 3.0 m min^{-1} have been used. Torch passed over the sample in its centre. During some part of the cycle time period the torch moves over the sample surface (heating time) and during the rest of the cycle it moves away from the sample to the dead point (cooling time). The number of 40 cycles has been used.

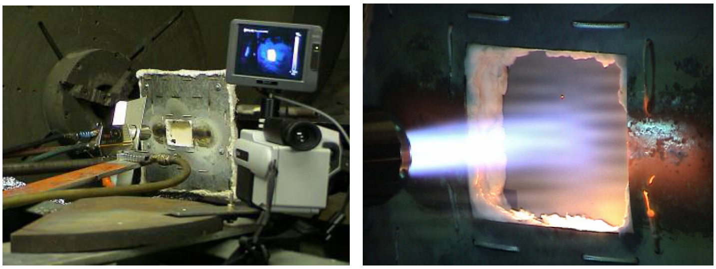

Figure 1: Experimental setup of TBC dynamic thermal loading tests.

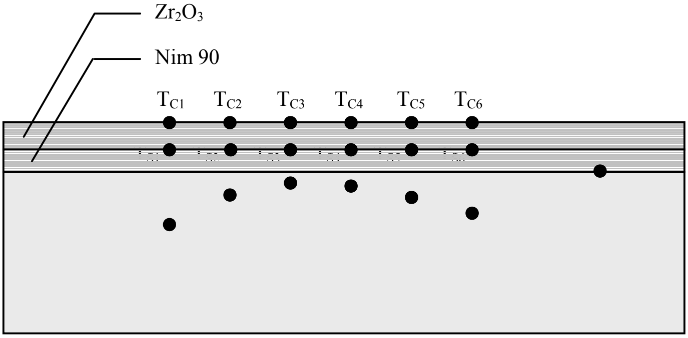

Figure 2: Position of measured and computed temperatures inside the sample.

Temperatures inside the sample have been measured by the built-in thermocouples. Six thermocouples (TC1 – TC6) were in the substrate in various depths under the surface and one (TC7) was on barrier-substrate interface (fig. 2).

The process of the sample thermal loading has been monitored by a digital infra-red camera. The recorded data have been used for the analysis of sample surface temperature distribution during the torch motion.

Table 1: Real thickness of thermal barrier layers.

Layer	Thickness
Steel 15330	20 mm
ZrO_2	0.192 mm
Nim 90	0.162 mm

Table 2: Real depth of thermocouples under surface.

Thermocouples	Depth
TC1	3.7 mm
TC2	2.0 mm
TC3	0.8 mm
TC4	1.4 mm
TC5	2.7 mm
TC6	4.3 mm

3 Theory

3.1 Mathematical model

The model has been designed to simulate reaction of the TBC-substrate structure during thermal shock. Perfect contact between individual layers of the thermal barrier and substrate is supposed.

Non-stationary heat conduction in individual layers of the thermal barrier and the substrate is assumed by the heat transfer equation. Thermal loading effect of the moving torch is simulated as a heat flux boundary condition on the TBC surface.

3.2 The Application of the Exodus method

The theoretical background for the Exodus method [1] is presented in [7, 8]. We specifically apply the method to the heat transfer equation in rectangular solution region. We use a 2D simulation model.

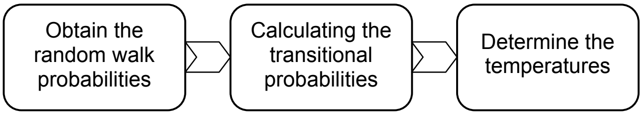

Figure 3: Scheme of solving a problem by the Exodus method.

To apply the Exodus method in finding the solution it usually involves the following three steps [9] as we can see in fig. 3:

1) First, the random walk probabilities are obtained from the finite difference equivalent of the partial differential equation describing the problem.
2) Second, the Exodus method is used along with the random walk probabilities in calculating the transition probabilities.
3) Finally, the temperature at the point of interest is determined from the transition probabilities and the boundary conditions.

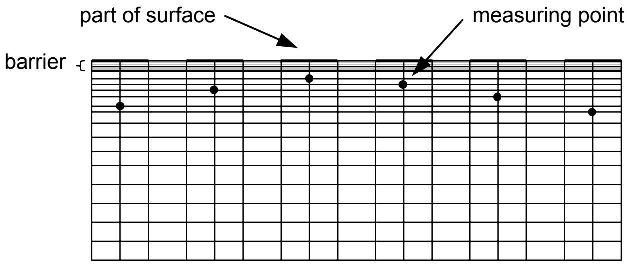

Figure 4: Computing mesh with distinguished input nodes and parts of surface.

The Exodus method solving indirect problem can determine only the same number of unknown temperature evolutions as the number of input temperature evolutions. Thus we split the surface to parts, corresponding to measuring points (fig. 4). Temperature and heat flux are evaluated for each part of surface.

3.2.1 Determining heat flux

Heat flux on the surface is determined from the temperature difference on the surface and in some depth δ, for example 10^{-5} m, below the surface. First, temperature is set on the normal mesh and further on the mesh, where the surface nodes are shifted as we can view on fig. 5.

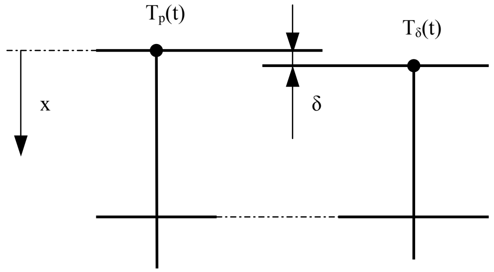

Figure 5: Schema of computing heat flux.

Heat flux is computed from this equation

$$q = \left(T_p(t) - T_\delta(t)\right) \cdot \lambda \cdot \delta^{-1} \quad (1)$$

3.3 Computer simulation

The presented computer simulation model is built to solve the indirect problem of the determination of temperature and heat flux intensities on the surface of the coated material. Inputs of the model there are the time evolution of temperature measured in six internal nodes and initial temperature, as outputs there are time evolution of surface temperature and surface heat flux. The original measured temperatures are processed in order to remove noise because during solving the indirect problem a small signal noise causes a big noise in the output. The input temperature time evolutions can be seen in fig. 6.

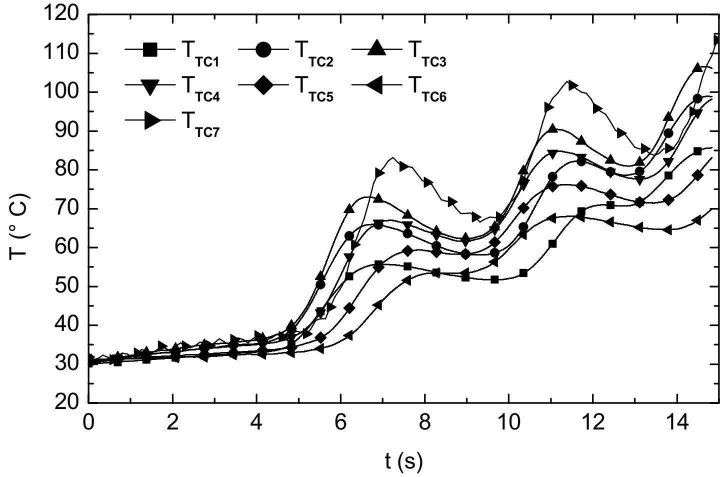

Figure 6: Input temperature time evolutions from thermocouples.

Thermophysical material properties and thickness of layers used in calculation are listed in Table 1 and Table 3. Sample is embedded thermocouples in various depths. The real depths of thermocouples are shown in table 2.

Table 3: Material properties of thermal barrier layers.

	ZrO_2	Nim 90	Steel 15330
Thermal conductivity (W m^{-1} K^{-1})	1.6067	12.5148	40.0475
Thermal capacity (J kg^{-1} K^{-1})	488.9739	278.3659	430.9387
Density (kg m^{-3})	5645	8254.4	7806.9

The temperature time evolutions determined by the Exodus method as the result of the inverse problem are used as the boundary condition in the FEM model based on the COSMOS/M system. Then we solve direct problem of heat propagation in multilayer TBC. Results of this model are compared with the measured temperatures.

4 Results

4.1 Simulations of TBC behaviour

The Exodus stochastic simulation method has been used to determine the intensity of heat transfer to surface during the first pass of the torch over the sample surface. The corresponding temperature evolution from embedded thermocouples at various depths under the substrate surface is shown in figure 6.

The resultant values of temperatures on the TBC surface and heat fluxes to the barrier are shown on fig. 7. Temperature time evolution on coatings-substrate boundary and heat transfer intensity to the substrate are plotted in fig. 8.

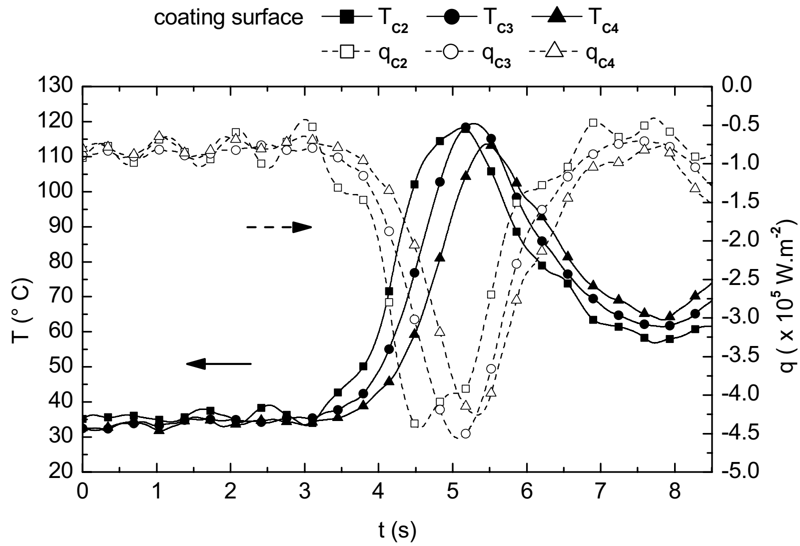

Figure 7: Time evolutions of temperatures and heat fluxes on TBC surface.

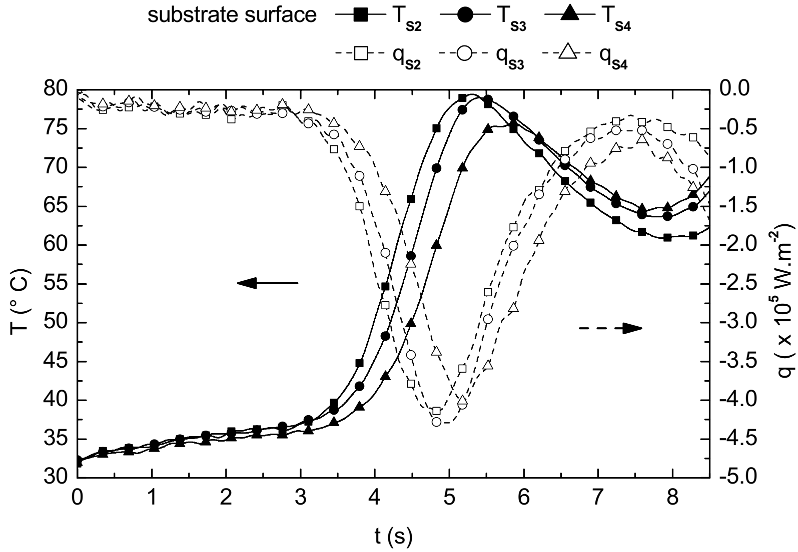

Figure 8: Time evolutions of temperatures and heat fluxes on coatings-substrate interface.

Maximum temperature 120 °C was reached in the first pass on the coating surface, which is the increase about 88 °C above the initial temperature 32 °C. The maximum heat flux to the thermal barrier surface is $4.5 \cdot 10^5$ W m^{-2}. The maximum temperature on the coating-substrate boundary is 80 °C in the first pass. The maximum heat flux to the substrate is $4.2 \cdot 10^5$ W m^{-2}.

The maximum of heat flux is reached before the maximum of temperature. The value of heat flux to the substrate is slightly smaller then to the coating, because a fraction of heat applied to heating up the TBC material. The maximum of temperature on the coating-substrate interface is smaller then on the coating surface, about two-thirds of the value on the coating surface.

4.2 Comparison with measurement

Comparison of the computed time evolution of temperature on the TBC surface with the measurement provided by IR camera is shown in fig. 9. There is a good agreement considering the temperature between peaks. Differences can be found in peaks where the maximum of measured temperatures is greater than computing one. This difference is caused either especially caused by a 2D model geometry which neglects the heat transfer to the lateral sides and either by the measurement error (effect of torch combustion gas radiation, about a quarter of the difference).

The second comparison confronts the temperature time evolution on the barrier-substrate interface with the measured temperature from TC7. The maximum temperature of T_{TC7} was 80.5 °C. The temperature on the barrier-substrate interface computed by the Exodus method achieved maximum from 75 to 80 °C.

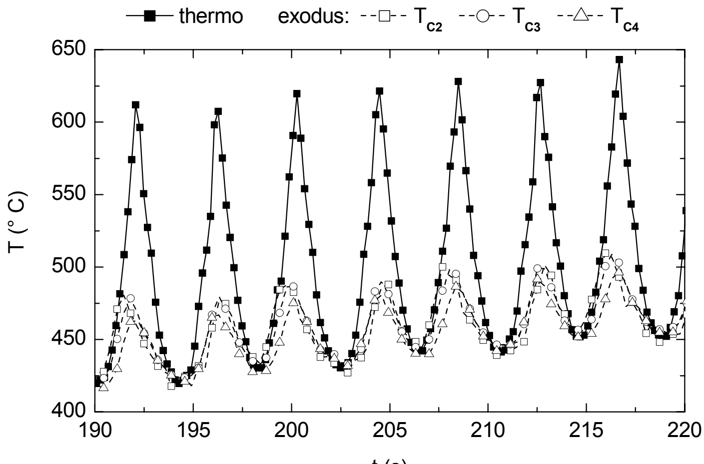

Figure 9: Comparison of computed temperature time evolutions on surface with thermography measurement by IR camera.

4.3 Comparison with FEM model

Results provided by the Exodus method have been also compared with results obtained by the finite element method. The FEM model based on the COSMOS/M FEA system used the results of the inverse problem computed by the Exodus method as the boundary conditions. Heat propagation in the multi-layer sample is solved as a direct problem and temperature time evolutions in measured points are compared with the original measured temperature evolutions. The comparison can be seen in Fig. 10, the differences between the measured and computed temperature in maximum are less then 5 °C in the first pass.

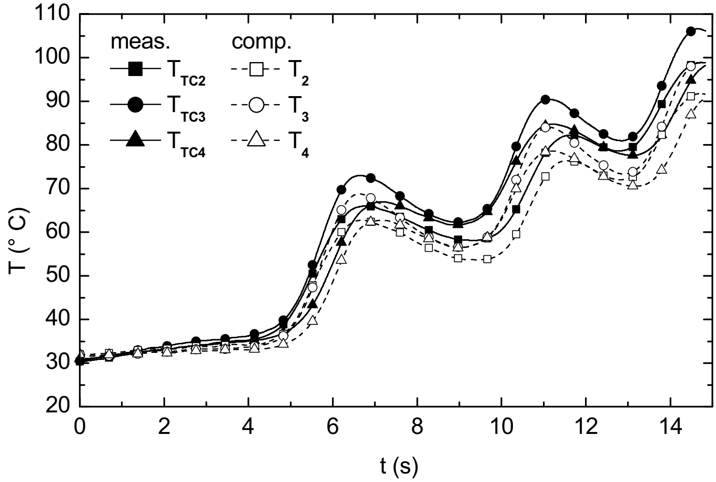

Figure 10: Comparison of measured temperature time evolutions with computed temperatures by FEM model.

5 Conclusion

The simulation model of the thermal barrier sample has been created. The experimentally obtained temperature evolutions at various depths and locations in the sample were used to find the heat transfer to the surface during thermal loading.

The Exodus method provides a relatively straightforward means of solving indirect problems. The method has been illustrated with typical problem of heat transfer in inhomogeneous solution region.

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