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# Finite element analysis of stress distribution in thermal barrier coatings

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ABSTRACT

A numerical simulation of crack development within APS TBC systems is presented. The TGO thickening and creep deformation of all system constituents is modelled. Two dimensional periodic unit cell is used to examine the effect of interfacial asperity on stress distribution and subsequent delamination of APS TBC. A study of cyclic loading and of creep of the base material on the stress distribution close to the asperity at the TGO/BC interface is made, revealing a small influence influence of both on the stress state in the thermal barrier coating system subjected to temperature loading. Cohesive zone elements at the oxide/ceramic interface model the development of the interfacial micro-crack. The finite element analysis shows that the development of the interfacial crack allows for a micro-crack formation within APS TBC. Subsequent TGO growth results in a tensional zone within the oxide layer. Linking of the micro-cracks at the interface and within TBC through TGO could lead to a coating delamination in the unit cell.



## 1. Introduction

During the last decade there has been an enormous effort to introduce single crystal and thermal barrier coating (TBC) technologies for the manufacture of high temperature components for advanced power generation gas turbines. One of the driving forces for this development is the desire to increase fuel gas temperatures, resulting in an improved thermal efficiency and thus making a primary contribution to the conservation of energy resources and to the limitation of $CO_2$ and other greenhouse gas emissions. Mostly for this reason, the use of thermal barrier coated Ni-based super-alloys for the thermally high loaded components will help to improve the gas turbine efficiency [1].

The potential of new generation single crystal super-alloys used for blade production is basically given by their superior creep and fatigue resistance up to 1000 °C [2,3]. The increase of fuel gas temperature in recent years has led to temperatures at the material surface reaching the values up to 1250 °C and a further temperature increase is envisaged. These thermal loading conditions can only be handled by a combination of modern cooling methods and protective coatings on top of the blades. In film cooling, the cooling air bled from the compressor is discharged through holes in the turbine blade wall or the end wall. The coolant injected from holes forms a thin thermal insulation layer on the blade surface to protect the blade from being overheated by the hot gas flow from the combustor. Typically, the holes are in diameter not bigger than 0.5 mm and are either normal to the surface or inclined at an angle of 15–30° [4–6].

Another technology allowing for an increase in turbines efficiency is high temperature protective coatings. Current protective coatings are two-layer systems, with a metallic, corrosion protective bond coat (BC, e.g. MCrAlY or PtAl) on the super-alloy and a ceramic thermal barrier coating (mostly Yttria stabilised $ZrO_2$) on top and in contact with the hot gas [7]. The thermal barrier coating provides a temperature drop of up to 200 °C due to its low thermal conductivity, which is enhanced further by the intentionally porous micro-structure. Fig. 1 demonstrates the reduction of temperature achieved by thermal isolation through TBC and inner cooling. The potential for a temperature reduction by TBC application, however, has not been fully exploited so far because in the case of failure the internal and external cooling air must be sufficient to keep the temperature in the structural material below the point at which failure occurs. To use the high potential of TBCs, the different aspects of exposure conditions and failure mechanisms must be understood and integrated into degradation modelling and life prediction.

A major weakness of TBC systems is the interface between the metallic bond coat and the ceramic TBC. At this interface an in-service degradation is observed often leading to a macroscopic spallation of the ceramic layer [8]. The interface regions undergo high stresses due to the mismatch of thermal expansion between BC and TBC. Additionally, growth stresses due to the development of thermally grown oxide (TGO) at the interface and stresses due to interface roughness are superimposed. Stress relaxation leads generally to reduced stress levels at high temperature, but can give rise to enhanced stress accumulation after thermal cycling resulting in early crack initiation at the bond coat/alumina interface and spallation failure afterwards [1,9]. One of the key issues of the present paper is to investigate

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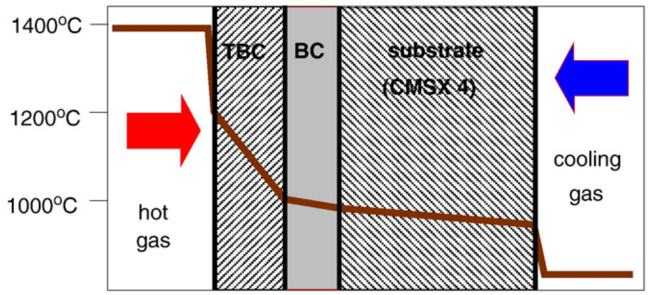


**Fig. 1.** Qualitative temperature distribution across the TBC system.

the influence of substrate creep upon stress distribution at the TBC/TGO interface and to examine whether only elastic substrate behaviour can be assumed during thermal loading. Moreover, the paper examines the effect of thermal cyclic loading and crack evolution within the TGO/BC interface.

Of particular interest in the present contribution is the experimental work on TBCs in which CMSX-4 super-alloy hollow cylindrical specimens were tested [7]. The specimens were plasma sprayed with yttria stabilised zirconia (APS TBC) on NiCoCrAlY bond coat. Experimentally determined data for APS TBC, TGO and BC creep [7,10,11] serve here as an input for material modelling of the constituents. The time-dependent model of CMSX-4 presented in [2,3] has been used. The oxidation process has been simulated by growth of thickness of TGO elements. The development of cracks at the TGO-BC interface has been simulated using cohesive zone elements. The results are next discussed in relation to the failure mechanism presented by Chang et al. and Freborg et al. [12,13].

## 2. The simulation scheme

There have been many attempts to numerically investigate stress development in TBC systems [9,12–24]. In most cases a 2D-unit cell representing a single asperity was used. The stress field around the asperity was supposed to be representative for the entire interface area. The resulting micro-cracks could subsequently link and thus

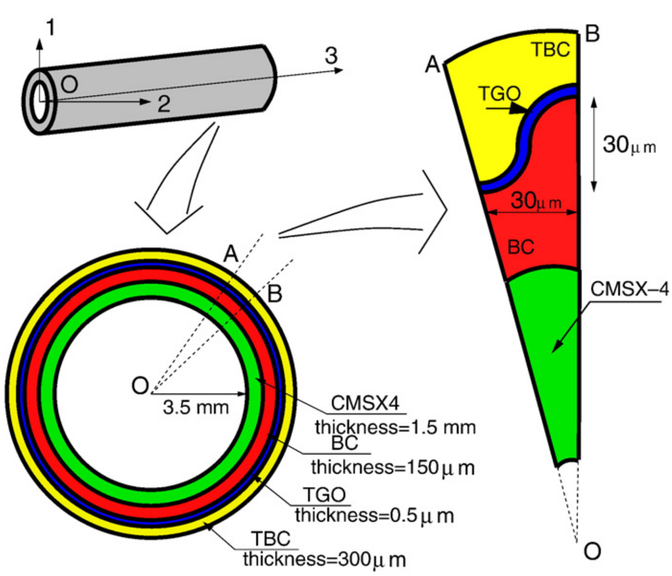


**Fig. 2.** The model of the cylindrical test specimen. The proportions of the layers in the figure do not resemble their actual dimensions.

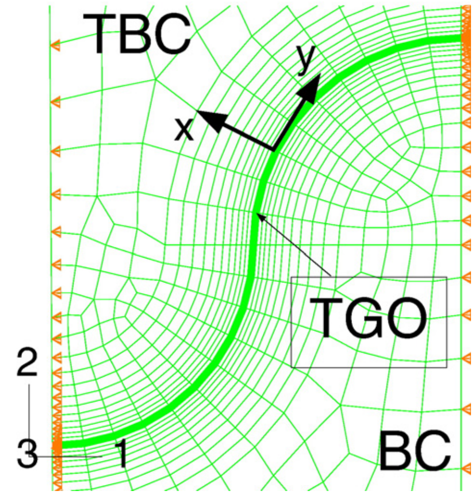


**Fig. 3.** Local coordinate system for the oxidation modelling. Boundary conditions on the edges of the unit cell.

form a crack crossing a number of asperities at a macro level. Using a unit cell approach this paper follows the multi-scale modelling concept.

### *2.1. The numerical model*

Fig. 2 illustrates the modelling concept. The test cylinder is sufficiently long compared to its diameter for the problem to be approximated by a two-dimensional plane-strain case. It has been assumed that the strain in the axial direction is uniform. As proposed in Fig. 2 the bond coat topography is idealised by circular segments within a unit cell. Symmetry of the problem allows meshing only one half of the undulation. The assumed boundary conditions put constraints on the displacement field in the cylindrical direction, only radial displacements are allowed to take place along lines OA and OB in Fig. 2 as schematically indicated on the finite element mesh in Fig. 3. The cylinder was subjected to cyclic temperature loading with homogeneous temperature distribution. A single loading cycle is presented in Fig. 4.

The bond coat, the thermally grown oxide and the thermal barrier coating are treated as elastic and viscous materials. Their mechanical properties are functions of temperature as listed in Table 1 (see [2] for the discussion of anisotropy of mechanical properties of CMSX-4). The value of temperature loading equal to 200 °C was chosen for the initial

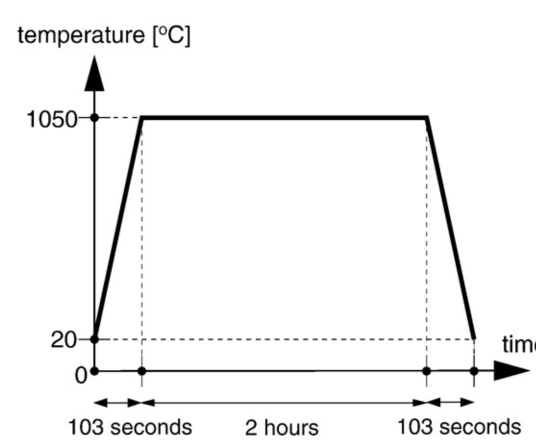


**Fig. 4.** Temperature profile during a single loading cycle.