Finite element modelling and damage evaluation of air plasma sprayed thermal barrier coatings

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Abstract.

The present paper describes the work done in order to establish a correlation between observations of thermal barrier coating (TBC) damage in an air-plasma sprayed TBC system and modelling of the delamination and spallation process that over time will degrade the TBC system. By inspections of cross-sections of TBC’s on ex-serviced gas turbine components, it will be possible to establish preferred crack paths, and, verify that assumptions made during the modelling and experimental verification stages will be valid for different load / temperature combinations.

Previously, a crack growth approach has been adopted for TBC delamination and spallation. This approach assumes that the top coat (TC) / bond coat (BC) interface is the region of the TBC that will develop a delamination crack network.

In the present work it has been shown that the assumption of crack growth along the TC / TGO interface is valid unless the TGO growth rate is disturbed by formation of large mixed oxide clusters. The same is true for in-plane stresses, where a typical component load situation will cause interface spallation at the same oxide/oxide interface as was observed in the case of cyclic temperature load. In areas where high tensile strains are introduced, the coating will not delaminate and spall. Instead through-thickness cracks are introduced, i.e. TGO upper limit and maximum tensile strain criteria need to be adopted in addition to the Paris law approach.

Introduction

Thermal barrier coatings (TBC) are extensively used in applications where resistance is needed against high temperatures in aggressive environments. The most common application is gas turbines where TBC’s are frequently used [1-3]. Despite the large acceptance of using coatings in engines, a persistent problem is the lack of reliable coating lifing tools. Strain-based power law oxidation dependent models have been thoroughly investigated [4-6]. Another approach for assessment of TBC life is to adopt a fracture mechanical philosophy [7-9].
Damage development in thermal barrier coatings is a process where delamination cracks are typically initiated at the top coat / bond coat interface [10, 11]. Due to a combination of time at temperature and cyclic thermal loading, existing and newly formed delamination cracks will grow and coalesce [8, 12] during repeated thermal/mechanical cycles. The cracks will grow either at the interface or near the interface in the ceramic top coat depending on whether the thermally grown oxide at the TC/BC interface is the weak link or not [13]. External loads and the stress/strain induced by thermal mismatch also play significant roles in the damage development process and contribute to growth of delamination or segmentation cracks [14]. In the present work, a model has been developed, where delamination crack growth is assumed to be confined to a region at the metal / ceramic interface.

The current work aims at investigating criteria when the crack will grow either at the interface or in the top coat. By evaluation of material exposed to engine conditions and material exposed to furnace cycling, the feasibility of using a previously proposed spallation fatigue life model [8] is discussed.

**Experimental details**

**Material** The material system used in the present furnace test series is sprayed onto rectangular coupons (30x50x5mm) of Haynes 230 nickel-base superalloy. On the Haynes 230 base material (BM) a NiCoCrAlY bond coat (BC) and an Yttria stabilized Zirconia (YPSZ) top coat (TC) was applied by air plasma spray (APS) technique. The as-manufactured material system is shown below, Figure 1. The same coating system has been applied to combustor and turbine stator components and evaluated after service exposure.

![Figure 1. As-manufactured thermal barrier coating system of the type used in the present study.](image)

**Material testing and characterization** Thermal cyclic fatigue (TCF) testing has been conducted in a furnace, where temperature is cyclically varied between 100 and 1100°C. This is achieved by moving the specimens between the furnace and a cooling nozzle utilizing compressed air as cooling media. The thermal cycle includes a dwell time of 60 minutes in the furnace.

Components exposed to engine conditions have been used as reference material. Five different sections have been cut and evaluated, where the locations are chosen so that different loading conditions are compared. Details are given below in Table 1.

**Damage development in thermal barrier coatings** Generally speaking, damage development in TBC systems will be dependent on cyclic thermal and/or mechanical loading. Previous work has indicated an effect from stress concentration at edges, metal oxidation, surface curvature, interface roughness and TC sintering [15-17].
**In-plane loading** During service, a mechanically stressed coated component can exhibit transverse cracking in contrast to the more frequently observed delamination crack type. A large in-plane load (and correlating strain) will cause the material to crack through the ceramic thermal barrier if the applied strain is larger than the fracture strain for the material in question. Mechanical loading as well as thermal cycling with high heat input (burner rig testing) have shown this type of damage development. The cracks in this case can penetrate the entire coating thickness [18, 19].

<table>
<thead>
<tr>
<th>Position</th>
<th>$T_{meas}$</th>
<th>$\sigma_{max, principal}$</th>
<th>Delamination location</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>-</td>
<td>-</td>
<td>TGO / TC interface. Black failure, interface crack</td>
</tr>
<tr>
<td>B</td>
<td>+</td>
<td>+</td>
<td>BC / TGO interface $\rightarrow$ TGO / TC interface $\rightarrow$ TC kink crack</td>
</tr>
<tr>
<td>C</td>
<td>++</td>
<td>-</td>
<td>TGO / TC interface $\rightarrow$ TC segmentation (multiple) kink cracks</td>
</tr>
<tr>
<td>D1</td>
<td>-</td>
<td>+</td>
<td>through-thickness cracking (due to high in-plane stress/strain state)</td>
</tr>
<tr>
<td>D2</td>
<td>-</td>
<td>+</td>
<td>TC failure (white failure), TC crack</td>
</tr>
<tr>
<td>E</td>
<td>--</td>
<td>-</td>
<td>Intact, no delamination</td>
</tr>
</tbody>
</table>

**Mechanical and / or thermal cyclic loading** Cyclic thermal or mechanical loads acting on a coated structure will, as previously discussed, cause gradual degradation of the interface between bond and top coat. Eventually, the coating will fail due to spallation where parts of the coating will experience buckling and local flaking if delaminations are present internally [20, 21]. For assessment of interface delamination crack growth, a Paris approach was suggested [8]. In this type of approach the material is considered to contain defects already in the as-sprayed state. Below in Figure 2 are shown the different delamination crack patterns likely to be found in a TBC system [8].

**Oxidation** The coating degradation due to oxidation is frequently discussed in open literature [22-26]. By continuous formation of oxides, the interface stress state is gradually increased. With time, the oxide will form a weak link between BC and TC. If the oxide is allowed to grow thick, isothermal experiments show that one single thermal cycle will be enough to completely separate the top coat from the underlying base material / bond coat. The change from alumina as a preferred TGO into formation of chromia and mixed Ni, Cr, Co, Al-oxides (spinel) is a phenomenon known to indicate that aluminium is depleted and that the TBC life limit is reached [22, 25, 26].

**Spallation life** A TBC spallation life model formulation was previously developed [8] for thin thermal barriers. The basic assumptions were that the model should be on Paris law for crack growth and that the damage is confined to a well-defined material volume at the TC/BC interface. Delamination typically will take place at the TC / TGO interface; either as interface cracks TC/TGO or TGO/BC, interface-near TC cracks or as kink cracks, where the crack typically would be initiated at the TC/TGO interface with propagation partially at the interface, partially in the ceramic TC close to the interface. If the crack is not confined to the immediate TC/TGO interface, it is also of great importance to understand how large region of the top coat is actively affected by delamination crack growth.

**Delamination and spallation** Development of delamination damage has been discussed by Brodin and co-workers [8]. The general observation has been that the damage development initially is rapid. With increased number of cycles the growth rate decreases, and, for thin TBC’s, a plateau is reached where damage development is retarded. Available data from other research groups utilizing non-destructive measurement techniques [12, 27] indicate that the plateau is not as significant and that the damage development is more continuous. This is also seen in our test data where thicker TBC’s will be inferior to thin TBC’s regarding thermal cyclic life, if TBC’s of a given BC/ TC composition are exposed to a fixed load situation [28, 29]. One way to quantify damage development was
proposed in the work by Brodin [8]. The method is to sum damage within a certain zone in the TC measured from the TC/BC interface. The damage, consisting of interface cracks in the BC/TGO/TC area, interface-near cracks in the TC and kink cracks in TGO and TC, will be normalized by an interface length over which the measurement is being performed. The corresponding damage parameter $D$ is then defined as [8]:

$$D = \frac{\sum_l l_{i}^{TGO} + \sum_j l_{j}^{TC} + \sum_k l_{k}^{TC/TGO}}{L_m}$$  \hspace{1cm} (1)$$

where $D$ is the damage parameter $0 < D < 1$, $L_m$ is the total evaluated interface length projected onto a plane parallel to the surface, $l_{i}^{TGO} (= l_{1})$ are interface cracks at the thermally grown oxide, $l_{j}^{TC} (= l_{2})$ are interface-near cracks and $l_{k}^{TC/TGO} (= l_{3} \text{ and } l_{4})$ are kink cracks as shown below, Figure 2.

Figure 2. Possible damage patterns in thermal barrier coating systems.

A schematic graph of damage evaluation in a TBC system with a weak TGO interface is shown below, Figure 3. In real cases the damage is never allowed to reach $D = 1$, since this would indicate a large-scale spallation and risk for component functionality. Therefore, for every coating system a material dependent value $D_{crit}$ must be applied, such that the coating system is considered to be failed when a damage level $D$ is present according to $D = D_{crit}$, where $D_{crit} < 1$. With the present evaluation philosophy, $D_{crit}$ and corresponding spallation life, $N_s$, is considered as the end of the plateau in Figure 3, before onset of stage IV leading to final failure, $N_f$. From experimental observations [27], the required defect size leading to spallation will be in the range of 3-5mm.

**Damage modelling** Stress levels and stress intensity factors at the coating system interface are typically not measured directly, but computed by finite element (FE) analysis. In the present work, a strategy is chosen where an elastic computation is performed from service (maximum temperature down to engine stop (or minimum temperature in a furnace cycle). Hence, it is assumed that the damage occurs at low temperature, where the stresses at the undulating TC /BC interface will cause local separations, delaminations. It has been assumed that the damage can be confined to the TC / BC interface and that cracks not necessarily have to grow in a pure modus I case. Instead, the interface will enable crack growth under a mixed modus I / II load situation. For evaluation purposes, an idealized geometry was used. A sinusoidal curve was chosen to represent the TC/BC interface. By choosing different wavelength/amplitude relations it will be possible to correlate surface roughness to stress intensity at a crack tip. In the FE model a crack was implemented at the TGO/TC interface. By sequential increase of the crack size, fracture mechanical data are retrieved for small delaminations up to complete interface spallation as shown below in Figure 4. In the model, cracks are introduced at neighbouring interface ridges. By doing so, stiffness at the interface will better represent the situation in an actual TBC system. The material behaviour of all
components in the TBC system during the cool-down from a stress-free state at maximum temperature is assumed to be linearly elastic. Temperature decreases rapidly, and the time at high temperature during cool-down is therefore not long enough to allow plastic deformation to take place. The results from our fracture mechanical modelling work indicate that the initial crack growth takes place in a $K_I$ dominant loading situation. As the damage level $D$ increases, the stress intensity state becomes more complicated with larger influence of $K_{II}$. As the damage level reaches spallation failure ($D \rightarrow D_{crit}$) the stress-state at the crack tip is translated into a $K_{II}$ modus. The driving force is reduced with increased $D$ and enables delamination cracks to be present over long time periods without causing spallation. The approach is more closely discussed elsewhere [8].

![Figure 3. Schematic damage development in thermal barrier coatings. Initial damage $D_0$ and corresponding number of cycles $N_0$ to onset of crack growth. Coating life is considered to be consumed at $D_{crit}$ after spallation life $N_s$ is reached. Complete failure $D_f$ due to spallation of the coating system ($D = 1$) is defined as $N_f$.](image)

**Fractographic results**

Evaluation of TBC-coated components has been done and delamination results are presented below. For comparison, results are included from thermal cyclic tests on corresponding material exposed to a test rig environment, ambient air and cycling from 100°C up to 1100°C.

**Damage in components** Evaluations of damage in regions with planar interfaces indicate that the damage mainly is a black failure type under high temperature. In the case of areas with high stress and high stress together with high temperature, the failure mode appears to be a mixed black / white delamination. Figure 5 through Figure 10 show typical microstructural observations in the present cases. Delamination damage is indicated by arrows in each picture.

![Figure 4. Calculated stress intensity factors $K_I$ and $K_{II}$ for a thin (0.3mm TC) air plasma sprayed thermal barrier coating of the type used in the present study. Left: comparison of $K_I$ (dashed lines) and $K_{II}$ (solid lines) for a given surface roughness. Right: Influence of surface roughness on stress intensity factor $K_I$.](image)
Figure 5. Damage in a low temperature, low stress region. Location “A” as referenced in Table 1.

Figure 6. Damage in a high temperature (T < ideal design temperature), high stress region. Location “B” as referenced in Table 1.

Figure 7. Damage in a high temperature (T > ideal design temperature), low stress region. Location “C” as referenced in Table 1.

Figure 8. Separation (through-thickness cracking) damage in a low temperature, high stress region. Location “D1” as referenced in Table 1.

Figure 9. Delamination (white) in a low temperature, high stress region. Location “D2” as referenced in Table 1.

Figure 10. Undamaged (no delaminations), ex-serviced material. Low service temperature. Location “E” as referenced in Table 1.
**Damage development in reference test material** For model calibration purposes, thermal cyclic fatigue testing has been performed and reported [8, 28, 29]. Corresponding damage patterns are shown below, Figure 11. Damage is confined to the TC/BC interface (black or black/white cracks).

![Figure 11. Damage patterns resulting from TCF testing. Black fracture (left) and mixed black/white kink crack (right) shown in figure.](image)

**Discussion**

In the reference test material, black fracture is commonly found in coatings where the alumina level becomes exhausted. If the TGO is dense and consists of alumina, the crack pattern will be of black plus kink type. This is in correlation with the findings by Renusch et.al. [30] where it was stated that aluminium depletion is linked to formation of thick oxides and TGO cracking. In engine-exposed coatings, a similar situation is observed in the case where a high temperature low stress situation causes multiple delamination cracks to form in a thick TGO and, hence, the TGO acts as a weak link. As previously discussed [22, 25, 26], due to aluminium depletion oxide morphology will be unfavourable. The lack of aluminium leads to increased oxidation rate. Consequently, a thick TGO causes the interface stress-state to be higher compared to a dense TGO after corresponding time.

Correlating the microstructural damage type to temperature and stress level shows a trend where presence of high temperature together with high mechanical stress initiates a mixed black/white failure. Presence of only stress causes the failure to shift into a white delamination failure where the interface will be stronger compared to the TC. Damage in the TC will probably initiate early and unload the interface to some extent. If moderate stress and temperature are applied, the TGO growth will gradually increase the stress state at the interface. With time, the moderate stress/temperature level can, as shown in the present work, cause small separations at the TC/BC interface in analogy with what is assumed according to modelling work [14, 20, 21].

Segmentation cracking in areas with high in-plane loads gives a situation corresponding to the damage described by Quian et.al. and Liu et.al. [18, 19]. Experimental work by Renusch [30] indicates that a critical strain level is expected to be in the range of 1% in the as-sprayed condition. Data in the work by Renusch show that this level will drop significantly over time.

A comparison between results from furnace cycling and engine exposed material indicates that damage patterns are similar and that the modelling approach chosen are suitable. If a model only incorporates interface cracks, limits must be put on the stress level, since increased stress will cause a shift from interface to TC failure.

**Conclusions**

An air plasma sprayed thermal barrier coating system was exposed to engine conditions and evaluated with respect to delamination and spallation damage. Findings indicate that multiple
damage types are found in a component and that a fatigue life model needs to take several degradation mechanisms into account. Depending on temperature level and external stresses the delamination pattern will change from interface TGO delaminations in the case of high temperature over to ceramic white failure if a high stress level is included. An excessively high in-plane strain level will cause the coating fail due to through-thickness cracking.

Comparing fracture patterns from components and cyclic furnace tests reveal that the damage development in the components and the furnace tests are similar. A higher degree of mixed black/white cracks are found in the furnace cyclic test series. Regarding life formulations, if the fracture is assumed to be contained at the BC / TC interface, constraints are needed on maximum service temperature and maximum in-plane strain level in the life prediction model.

References