Simulation of crack propagation in thermal barrier coatings

Martin Bäker

Institut für Werkstoffe, Technische Universität Braunschweig, Langer Kamp 8
38106 Braunschweig, Germany, e-mail: martin.baeker@tu-bs.de

ABSTRACT. *Thermal barrier coatings are used to protect turbine blades from the high temperature of the process gas inside a turbine. They consist of a bond coat which protects the substrate from corrosion and of a ceramic top coat with low thermal conductivity. During service, an additional oxide layer forms between bond coat and top coat. Experimentally, it is known that these layers fail by spallation when the oxide layer exceeds a critical thickness of about 10 micron. Finite element simulations show that the roughness of the interface between top and bond coat is crucial for determining the stress state. Lifetime models have been inferred that assume that cracks form in the peak positions at small oxide thickness and propagate when the oxide layer grows.*

In this contribution, a two-dimensional finite element model of crack propagation in this system is presented. Since the cracks propagate near a material interface, standard tools of fracture mechanics for predicting the crack propagation direction are difficult to apply. This problem is circumvented by propagating short "test cracks" in different directions and optimising to find the crack direction with the maximum energy release rate. It is shown that the energy release rate of cracks initiated at the peak position strongly depends on the creep properties of the TBC and the TGO. For creep-soft materials, the energy release rate is small, but increases during crack growth. Implications for the lifetime of TBCs are discussed.

1 INTRODUCTION

Thermal barrier coatings are widely used in gas turbines to protect turbine blades from the extremely high temperatures of the gas in the combustion chamber. Since increasing the service temperature of gas turbines is desireable to increase their efficiency, it is important to fully understand the behaviour of thermal barrier coating systems. However, thermal barrier coatings fail after some time, for reasons that are still not fully understood.

A thermal barrier coating system comprises several parts: The substrate, usually a nickel-base alloy, is first coated by a so-called bond coat which has a two-fold purpose. On the one hand, the bond coat serves as corrosion protection layer, on the other hand, it provides the surface roughness necessary for the adhesion of the thermal barrier coating (TBC) itself, which is made of Zirconia and applied by plasma spraying. During service, oxygen diffuses through the thermal barrier coating and oxidises the top region of the bond coat, forming an oxide layer, called thermally grown oxide or TGO. Experimentally,

it is known that thermal barrier coatings fail by spallation when a critical TGO thickness, usually about $10\,\mu\mathrm{m}$, is reached. Spallation is driven by microcracks that form at or near the TGO/TBC interface and coalesce [1].

To understand the failure behaviour of this system, it is necessary to analyse the stress state. Stresses at the interface are due to the differences in the coefficient of thermal expansion and to growth stresses that are induced by the growing TGO. Finite element simulation, for example in [2, 3], show that the roughness of the interface plays a crucial role. If the TGO is thin, "peaks" of the rough interface are under tensile stress. With growing TGO, the stresses shift and the tensile region moves to the valley position. From this, a lifetime model has been inferred where microcracks form at the peak positions and propagate to the valley position when the TGO grows.

However, these lifetime models so far have only looked at the stress state. If a crack forms, its presence changes the stress state, and this effect has so far not been studied. The reason for this is that crack propagation simulations in this system are problematic. Due to the presence of the interface and due to possible plastic deformation in the bond coat (and at high temperature also in the other materials), standard criteria to predict the direction of crack propagation (like the J-integral) are difficult to apply.

In this paper, a simple finite element tool is used to study this problem. The direction of crack propagation is calculated by propagating small test or trial cracks from the current crack tip and determining the direction of crack propagation by maximising the energy release rate. This method has the obvious disadvantage that it is computationally expensive, but since the crack propagation is actually performed in a finite element simulation, the energy release rates are available regardless of the complications discussed above.

The paper is structures as follows: In the next section, the method of trial crack propagation is explained in more detail and is studied for one verification problem. Afterwards, the finite element model of a TBC system is presented and some results of crack propagation studies are stated. The paper closes with an outlook and some thoughts on how the results affect the understanding of TBC lifetime.

2 CRACK PROPAGATION USING TRIAL CRACKS

2.1 Propagating trial cracks

The trial crack propagation algorithm is discussed in detail in [4, 5]. Consider a situation with an initial crack in a complicated stress field. We assume that the crack propagates in the direction where the energy release rate is maximum. In two dimensions, determining the angle of propagation is a one-dimensional optimisation problem. To solve it, several finite element calculations, are performed that propagate a trial crack by a fixed distance δa. The energy release rate is calculated for each simulation by comparing the stored elastic strain energy at the beginning and the end of the crack propagation step. To find the optimum crack direction, a Brent algorithm, described in detail in [6], is used. This

algorithm starts with a simple search to find a local maximum that is enclosed ('bracketed') between two other values and then refines the maximum position by decreasing the size of the bracketing interval. Calculation stops if the maximum is bracketed with a pre-defined precision. Usually, 6–10 trial crack calculations are sufficient to calculate the crack direction with an accuracy of 1–2°. After the optimisation has finished, the calculated maximum energy release rate can be compared with a critical value to see whether the crack would actually propagate. If it does, the configuration with the optimum crack direction is chosen as the starting point for the next crack increment.

Because the direction of the trial cracks is arbitrary, a remeshing of the geometry is needed for each trial crack calculation to ensure that the crack can travel exactly on the nodes between elements. After remeshing, the solution has to be interpolated from the old to the new mesh using the `Map solution` option of Abaqus [7]. This interpolation steps adds some inaccuracy, making it necessary to use a rather fine mesh.

2.2 Validation and verification of the procedure

To test the procedure, different examples have been studied, see [4, 5]. Here we present the well-known case of a crack loaded in mixed mode as verification example. Several criteria exist to calculate the crack propagation direction of a crack that is loaded in mixed mode or in pure mode II [8]. Frequently used are the maximum circumferential stress criterion, the maximum energy release criterion, or, for nonlinear problems, the J integral.

The chosen configuration for this problem consists of a quadratic plate with edge length $100\,\mathrm{mm}$ and an initial crack that extends through half of the specimen, see the inlay of Figure 1.

Load was applied by displacing the left and right side of the specimen by a fixed amount and then propagating the trial cracks. The displacement boundary condition was varied so that different values of K_I and K_II (which were determined using the postprocessing features of ABAQUS [7]) were obtained.

Figure 1 shows the calculated kinking angle as a function of $K_\mathrm{II}/(K_\mathrm{I} + K_\mathrm{II})$. The figure also shows the kinking angle predicted directly from the calculated stress intensity factors using the maximum energy release rate criterion [7], based on results shown in [9]. As can be seen, the agreement is acceptable, with the largest error being 3%.

3 APPLICATION TO THERMAL BARRIER COATINGS

3.1 Finite element model of a TBC

The model geometry (Fig. 2) is that of a solid cylindrical disk which is thought to be infinitely extended in its axial direction, almost identical to the model described in [3]. It comprises a superalloy substrate with a radius of $20\,\mathrm{mm}$, a bond coat with an average thickness of $150\,\mu\mathrm{m}$ and a thermal barrier coating of $150\,\mu\mathrm{m}$ average thickness. The

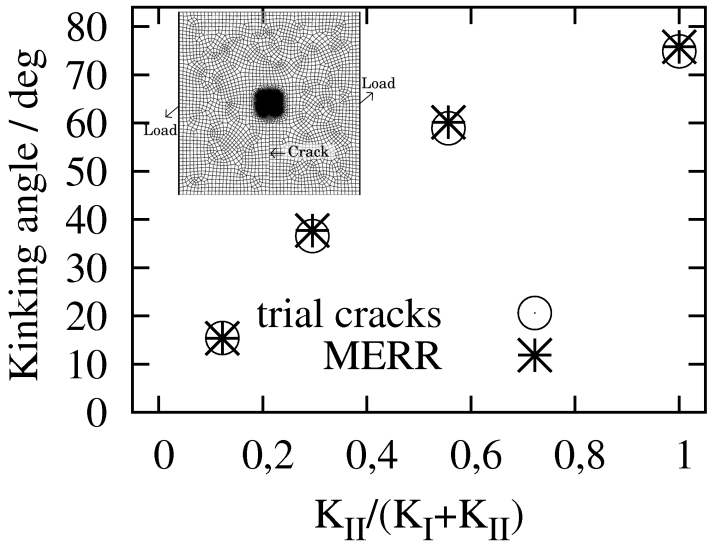


Figure 1: Calculated kinking angles in a mixed-mode problem. The kinking angle calculated by using trial cracks is compared to the value calculated using the maximum energy release rate criterion directly from the finite element model [7]. The inlay shows the finite element mesh.

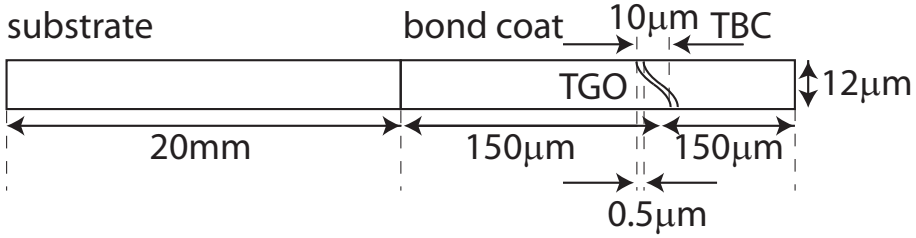


Figure 2: Model geometry. The model is cylindrically symmetric, with the axial direction being vertical.

interface region between bond coat and TBC is modeled with a sinusoidal geometry with a half-wavelength of 12 μm and an amplitude of ± 5 μm as shown in the figure. The initial TGO thickness was 0.5 μm. The model is constrained in the radial direction on the axis (at $r = 0$) in order to simulate a full cylinder with no inner hole. Nodes at the bottom of the model are constrained in axial direction, those on the top of the model are allowed to move in the axial direction, but the movement is constrained such that all these nodes must have the same displacement. Thus the model can be considered as a slice taken out of a sample

Table 1: Material properties used in the model, taken from [3]. Norton creep with a creep law $\dot{\epsilon} = A\sigma^n$ was assumed for bond coat, TGO, and TBC. Creep of TGO and TBC was varied within the ranges shown.

	Substrate	Bond coat	Oxide	TBC
Young's Modulus (20 °C) [GPa]	184	200	400	48
Young's Modulus (1100 °C) [GPa]	145	110	325	22
Poisson number (20 °C)	0.3	0.3	0.23	0.1
Poisson number (1100 °C)	0.3	0.33	0.25	0.12
CTE (20 °C) [K^{-1}]	$12 \cdot 10^{-6}$	$13{,}6 \cdot 10^{-6}$	$8{,}0 \cdot 10^{-6}$	$9 \cdot 10^{-6}$
CTE (1000 °C) [K^{-1}]	$16 \cdot 10^{-6}$	$17{,}6 \cdot 10^{-6}$	$9{,}3 \cdot 10^{-6}$	$12{,}2 \cdot 10^{-6}$
Creep exponent	no creep	3	1	1
Creep prefactor (1000 °C) [$\mathrm{MPa}^{-\mathrm{n}}\mathrm{s}^{-1}$]	no creep	$1{,}39 \cdot 10^{-7}$	10^{-6}–10^{-10}	10^{-5}–10^{-10}

that is very long and unconstrained in the axial direction. The geometry was meshed using approximately 15000 four-node elements with selectively reduced integration.

Material data can be found in table 1.

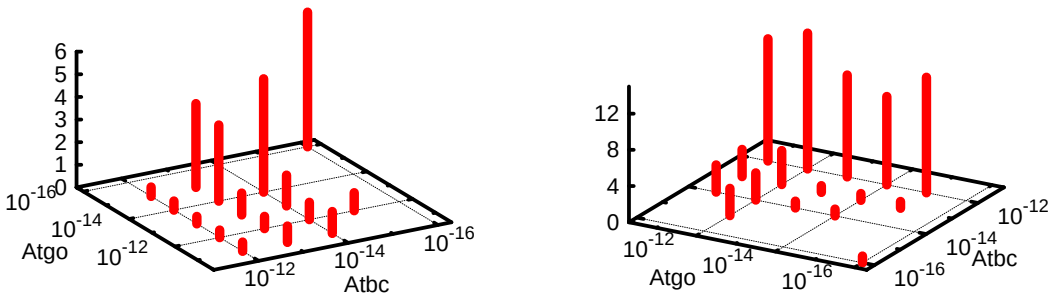
The model is thermally loaded, starting at a temperature of 20 °C. Within 60 s, it is heated to 1000 °C, held at this temperature for 120 s, and cooled back in another 60 s to 20 °C. There are two main causes of stress in the system: The TGO layer grows at hot time, thus increasing its volume. The extension of the TGO causes in its lateral direction puts the peak region of the sinusoidal region under pressure and the valley region under tension. This growth of the TGO is simulated using the `Swelling`-Option in ABAQUS. Details can be found in [3].

The second cause of stress is the mismatch of the coefficients of thermal expansion (CTE) between TGO, TBC, and bond coat. Due to creep at high temperature, the CTE mismatch stresses do not return to zero even without TGO growth. Depending on the thickness of the TGO, these stresses may be tensile or compressive at the peak position (and vice versa at the valley position), see [3].

After performing one thermal cycle, an initial crack of size 0.375 μm is initiated at the peak position of the TBC at the position of highest stress, directly above the TGO. Then, the crack propagation algorithm, described in the previous section, starts, using a trial crack length of 0.75 μm.

3.2 Results

As explained in the introduction, the Freborg model of TBC failure [2] assumes that an initial crack forms at the peak position of the TBC/TGO interface. It cannot proceed because it would enter a region of compressive stresses. The crack propagates to the valley position as the TGO grows.



(a) (b)

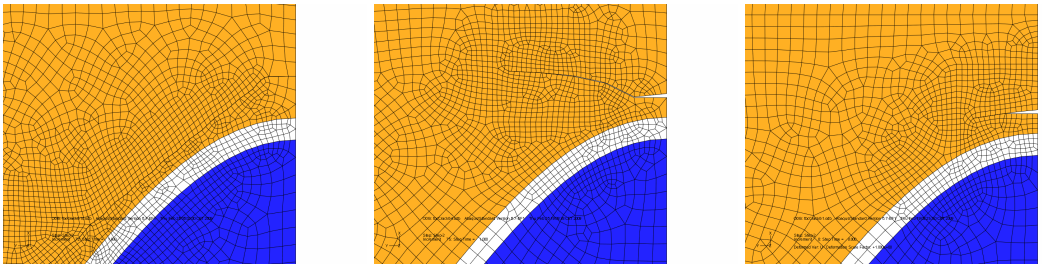
Figure 3: Crack propagation as a function of the creep strength of TGO and TBC. Left: Initial value of the energy release rate in $\mathrm{J/m^2}$. Right: Total accumulated crack length (in $\mu\mathrm{m}$) before the energy release rate becomes smaller the initial energy release rate. If the creep strength is low, cracks propagate throughout the simulation volume. Note the change in perspective relative to Figure 3(a)

To check this assumption, crack propagation simulations with a thin TGO layer were performed. A single thermal cycle was applied as described in the previous section and an initial crack was introduced at the TBC peak position. For the Freborg model to be valid, the energy release rate should become smaller as the crack propagates. If this were not the case, a crack would either not form at all or it would propagate to the valley position without TGO growth. It is quite clear that the creep properties of the TBC and the TGO are important in this as they crucially influence the stresses. Therefore, the creep prefactors (see Table 1) of TGO and TBC were varied by four or five orders of magnitude.

Figure 3 shows the results of the calculations. As can be seen from Figure 3(a), the initial energy release rate strongly depends on the creep strength and becomes very small when creep is fast. This suggests that cracks would not form or not propagate in soft materials. However, as Figure 3(b) shows, if cracks would form in these materials, they would stop only after having propagated almost or completely along the interface.

If, on the other hand, both materials have a large creep strength, the initial energy release rate is large initially but becomes smaller as the crack propagates. In this case, an initially forming crack could stop and might then propagate after the TGO has grown further. This case thus seems to be in agreement with the Freborg model.

Figure 4 shows the crack paths for three different values of the creep prefactors. Cracks are assumed to proceed until the energy release rate drops below its initial value, as this is the first possible moment where a crack could stop. In the case of a creep-soft material, the crack cannot stop and propagates along the interface. For medium and high creep strength, the crack path with the highest energy release rate is initially directed away from the interface. Further simulations are necessary to see whether the crack in this case would be able to proceed after the TGO has grown and whether the crack path agrees with experimental observations, moving along the interface.



(a) (b) (c)

Figure 4: Crack paths for three different values of the creep prefactors of TGO and TBC. The crack path is shown up to the position where the energy release rate becomes smaller than its initial value.

4 CONCLUSIONS

A method of calculating crack propagation using trial cracks has been presented. Although computationally expensive, this method is attractive in cases where standard crack propagation criteria are not easily applicable.

The method has been applied to the simulation of crack propagation in a thermal barrier coating system. After thermal cycling, crack propagation has been studied as a function of the creep strength of the TGO and the TBC. According to the Freborg failure model [2], cracks should be stopped by entering a region of compressive stress after being initiated in the peak region of the interface.

It was found that, if TGO and TBC are creep resistant, cracks once initiated would never stop as their energy release rate never drops below its initial value. For creep resistant materials, the energy release rate decreases below its initial value. However, the initial crack path does not agree with the expected path as it is directed away from the interface.

The values of the energy release rate become smaller when the materials are creep soft, as should be expected. Values are below $1\,\mathrm{J/m^2}$, so that it it doubtful that cracks would propagate at all in a creep-soft system. Therefore, a creep-soft TGO and TBC might be helpful in increasing TBC lifetime. Possible ways to achieve this are currently under study.

REFERENCES

[1] A. Rabiei, A. Evans (2000) *Failure mechanisms associated with the thermally grown oxide in plasma-sprayed thermal barrier coatings*, Acta Mat. **48**, 3963–3976

[2] A. M. Freborg, B. L. Ferguson, W. J. Brindley and G. J. Petrus (1998) *Modeling oxidation induced stresses in thermal barrier coatings*, Materials Science and Engi-

neering A, **245** , 182–190

[3] J. Rösler, M. Bäker, K. Aufzug (2004) *A Parametric Study of the Stress State of Thermal Barrier Coatings – Part I: Creep Relaxation*, Acta Mat. **52**, 4809–4817

[4] M. Bäker (2008) *Finite element crack propagation calculation using trial cracks*, Computational Materials Science,**43**, 179–183

[5] M. Bäker (2009) *Simulation of crack propagation in mixed mode and at bimaterial interfaces using trial cracks*, to appear in Computational Materials Science

[6] W. H. Press, B. P. Flannery, S. A. Teukolsky, W. T. Vetterling (1989) *Numerical Recipes*, Cambridge University Press, Cambridge

[7] ABAQUS Version 6.6, Simulia, Dassault Systemes

[8] D. Gross, T. Seelig (2006) *Fracture Mechanics*, Springer, Berlin

[9] M. Y. He, J. W. Hutchinson (1989) *Kinking of a Crack out of an Interface*, J. Appl. Mech. **56**, 270–278