# Design Geometry Optimization of Vertical Cracks in Thermal Barrier Coatings From Simulated Thermal and Mechanical Behavior

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Abstract: Turbine blades are coated with thermal barrier coatings (TBCs) to reduce operating temperature. TBCs experience stress from coefficient of thermal expansion mismatch with the bond-coat and substrate. Vertical cracks are thought to offer stress relief, but influence of crack geometry on TBC thermal and mechanical properties is not well understood. A twodimensional, steady-state model is employed to evaluate stress, strain energy density, and temperature as crack distance, crack width, and crack depth vary. Results differ with boundary conditions. When external forced convection is allowed in cracks, increased number and depth of cracks offer mechanical stress advantage but also increase both sample temperature and average stress. When forced convection is disallowed within cracks, TBC thermal performance is not strongly affected by crack distance. More frequent and deeper cracks reduce coating stresses. Optimization of crack geometries is a complex problem depending on expected operating conditions of the turbine blade.

**Keywords:** Thermal barrier coatings, yttriastabilized zirconia, vertical cracks, turbine blade

# **1. Introduction**

Thermal Barrier Coatings (TBCs) have long been used for high temperature applications, such as gas turbine blades. The purpose of a TBC is to reduce temperature across the thickness of the layer, allowing higher operating temperature and efficiency (Figure 1). Due to unavoidable coefficient of thermal expansion mismatch between the TBC, bond-coat, and substrate, stress occurs during temperature change and can cause TBCs to spall.



**Figure 1:** Thermal barrier coatings reduce turbine blade operating temperatures [5].

Experimental results show that vertical cracks within a TBC offer strain tolerance [1-5]. Some control over crack geometries through type and rate of coating deposition has been demonstrated (Figure 2) [3-4]. Influence of crack geometry on TBC thermal and mechanical properties is not well understood. COMSOL multiphysics modeling was used to consider how crack-to-crack distance, crack width, and crack depth influence performance characteristics of TBCs.



**Figure 2:** Comparison of (a) traditional plasma sprayed TBC (b&c) TBC with vertical cracks (d) EB-PVD TBC [1]

# 2. Numerical simulation

#### 2.1 Model description

COMSOL 4.2a "Thermal Stress" and "Heat Transfer in Porous Media" Modules were employed in this two-dimensional, steady-state simulation. A 1690  $\mu$ m SiC base representing a turbine blade wall is coated first with a 10  $\mu$ m environmental barrier coating (EBC) of mullite (3Al<sub>2</sub>O<sub>3</sub>•2SiO<sub>2</sub>) followed by a 200  $\mu$ m TBC of yttria-stabilized zirconia (YSZ). The YSZ is 7% porous as measured through SEM images of coatings from our research group, similar to other reported findings [6]. YSZ materials properties represent 8mol% YSZ operating at 1200 C [7-8].

Consistent with experimental observations from our group and others [3-4], vertical cracks are placed in the YSZ at varying crack density (90-800  $\mu$ m), width (4  $\mu$ m or 2  $\mu$ m), and depth (half-thickness or full-thickness). Crack characteristics are homogenous throughout the sample for each simulation.

## 2.2 Boundary conditions

External forced convection is applied to the top boundary, including cracks, to represent surrounding combustion gases. Internal cooling via turbine serpentine channels is modeled using external forced convection along the bottom SiC boundary. Velocities, pressures, and temperatures are informed through reported measurements of gas turbine blades [9]. Model sides walls are insulated. Model geometries and parameters are detailed in Figure 3.

A comparison with cracks exempt from forced convection is another aspect of this study. For these simulations, only the top surfaces of inter-crack blocks are subject to external forced convection from combustion gases.



Figure 3: COMSOL model of TBC-EBC coated turbine blade

#### 2.3 Measurements

Simulation measures include Von Mises stress, strain energy density, and temperature. Temperature range of the whole sample is considered. Stress and strain energy extrema and average are calculated for the TBC, EBC, and substrate. These values are also determined for both the YSZ-mullite and mullite-SiC interfaces. To reduce edge effects, interfacial measurements are calculated along the boundary lines but removed from each edge by three cracks. Larger crack distance models are expanded to accommodate this requirement.

# 4. Results and Discussion

## 4.1 Temperature

As illustrated by Figure 4, temperature drops markedly through the YSZ layer and stabilizes through the rest of the sample. This result is consistent with the known function of TBC coatings (Figure 1).



Figure 4: Temperature decreases rapidly through TBC layer

Temperature minima and maxima decrease with greater distance between cracks. Halfthickness cracks have lower extrema than fullthickness cracks, while differences between crack widths are negligible (Figure 5). These results imply that increased surface area through additional and deeper cracks exposed to forced convection from combustion gases reduce the effectiveness of the TBC layer.



Figure 5: Temperature vs. inter-crack distance

# 4.2 Stress and Strain Energy Density

For all reported analyses, stress and strain energy density show similar trends. Accordingly, stress findings are chosen to represent most of our results. Maximum stress within the YSZ increases with crack distance (Figure 6) but average stress decreases (Figure 7). The mechanical purpose of cracks – relief of coating stresses resultant from CTE mismatch – is reflected in the decrease in YSZ maximum stress and strain energy density. By contrast, more cracks allow more thermal energy, and therefore YSZ average stress and strain energy density both trend upward as crack distance decreases (Figure 8). The mullite layer generally enjoys greater stress relief through more cracks. Both the maximum and average stresses and strain energy densities for mullite increase with crack distance (Figures 6-7).

Interfacial stress between the YSZ and mullite suggest optimization between mechanical stress relief (prefers more cracks) and thermal stress (prefers less cracks) (Figure 8). Average YSZ-mullite interface stresses are lower for halfthickness cracks. The mullite-SiC boundary prefers less cracks. As with YSZ-mullite, the mullite-SiC interface shows lower stresses for half-thickness cracks (Figure 9).



**Figure 6:** Maximum stress for YSZ and mullite vs. inter-crack distance



Figure 7: Average stress for YSZ and mullite vs. inter-crack distance



Figure 8: Average YSZ-mullite interfacial stress vs. inter-crack distance



Figure 9: Average mullite-SiC interfacial stress vs. inter-crack distance

### 4.3 Modified boundary conditions

A second model is considered where forced convection from combustion gases is excluded from cracks. These analyses are restricted to half-thickness, 4 µm wide cracks. Sample temperature remains close to a no-crack model, indicating more ideal function of the TBC layer (Figure 10). Maximum stresses and strain energy densities for both YSZ and mullite trend similarly to the forced convection model. However, average stresses and strain energy densities for both YSZ and mullite layers remain nearly unchanged throughout a range of crack distances (Figure 11). For this approximately isothermal comparison, the mechanical benefits of increased number of cracks are appreciated without the deleterious accompaniment of additional thermal energy and stress. Our findings underscore the importance of determining boundary conditions specific to the environment operating and airflow characteristics of the target turbine blade in order to effectively optimize TBC crack parameters with this modeling method.



**Figure 10:** Temperature vs. crack distance for no external convection in cracks



Figure 11: Max and average stress vs. crack distance for no external convection in cracks

# 6. Conclusions

Crack geometry and model boundary conditions strongly influence performance characteristics of TBC-EBC coating systems for turbine blades. When convection within cracks is considered, the stress-relieving benefits of more cracks are offset by additional thermal stress. A regime of lower TBC-EBC interfacial stresses occurs as a compromise between these trends. Half-thickness cracks result in less heating and thus less interfacial stress than full-thickness cracks. When forced convection within cracks is ignored, the TBC behaves more ideally in decreasing sample temperature, while the stressreduction function of cracks is preserved. More

frequent and deeper cracks therefore reduce both maximum and average TBC and EBC stresses. Optimization of crack geometries in TBC-EBC systems is a complex problem and depends considerably on expected operating conditions of the turbine blade. Further simulation work on crack geometry and coating characteristics is ongoing.

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# 8. Acknowledgements

We thank Professor Daniel Cole for useful discussion regarding our COMSOL model.