FEM simulation of TBC failure in a model system

P. Seiler¹, M. Bäker¹, T. Beck², M. Schweda² and J. Rösler¹

¹ Institut für Werkstoffe (IfW), Technische Universität Braunschweig, Germany
² Institut für Energieforschung/ Werkstoffstruktur und -Eigenschaften (IEF 2), Forschungszentrum Jülich, Germany

p.seiler@tu-bs.de

Abstract. In order to study the behavior of the complex failure mechanisms in thermal barrier coatings on turbine blades, a simplified model system is used to reduce the number of system parameters. The artificial system consists of a bond-coat material (fast creeping Fecralloy or slow creeping MA956) as the substrate with a Y₂O₃ partially stabilized plasma sprayed zircon oxide TBC on top and a TGO between the two layers. A 2-dimensional FEM simulation was developed to calculate the growth stress inside the simplified coating system. The simulation permits the study of failure mechanisms by identifying compression and tension areas which are established by the growth of the oxide layer. This provides an insight into the possible crack paths in the coating and it allows to draw conclusions for optimizing real thermal barrier coating systems.

1. Introduction

Plasma sprayed thermal barrier coating systems are used on top of highly stressed components e.g. in gas turbines. They protect the underlying nickel-basis substrates from the high surrounding temperatures. A typical coating system consists of a nickel-basis substrate, the metallic bond-coat, and the thermal barrier coating (TBC). These coatings fail in service because of the thermally grown oxide (TGO) between the bond-coat and the TBC, and the complex load [1]. Furthermore, the interfacial roughness of the substrate and the creep properties play an important role in the failure mechanisms [2].

A model system was developed to reduces the influence parameters which leads to the spallation of the coating system. The model system contains of the MCrAlY bulk material Fecralloy which is in this case used as the substrate of the coating system. The TBC is applied directly to this substrate. Therefore, all influences of a nickel-basis substrate can be neglected and a system with reduced coating layers can be analyzed in order to draw conclusions for optimizing real thermal barrier coating systems.

To study the creep influence of the bond-coat material itself a second substrate was used in the model system: the slow creeping oxide-dispersion-strengthened (ODS) material MA956.

The TGO as the third layer in the system grows between the substrate and the TBC by oxygen that diffuses through the TBC. This is caused by the high porosity of the TBC and the high ionic diffusivity of oxygen [3]. The oxidation is an inward growth of α-Al₂O₃ [1]. The growth of the TGO promotes the failure of the coating system. Therefore, the growth stresses are examined.
2. FEM model

The geometry is almost identical to the model described in [2] and [4]. Fig. 1 shows a sketch of the system. It was generated by a C++ preprocessor for ABAQUS [5] and consists of CAX8RHT elements. All layers in the model are free of stress at the beginning of the simulation. The initial TGO thickness was varied between 1 µm and 7 µm. The temperature of 1000 °C was held for 2 h. The analysis of the stresses was performed at prominent positions at the interface (valley and peak positions in Fig. 1). The discussed stress values at this positions are the mean values of the radial stresses $\sigma_{11}$ at the integration points.

![Figure 1. Sketch of the model system with the marked valley and peak positions.](image)

The material parameters of the TGO and the TBC can be found in [2]. The measured parameters of Fecralloy and MA956 are shown in Tab. 1. The Poisson number $\nu$ and the thermal expansion coefficient $\alpha$ are the same as MCrAlY and can also be found in [2].

|                         | Fecralloy | MA956 |
|-------------------------|-----------|--------|
| Young’s modulus $E$, 20°C [GPa] | 148.6     | 148.6  |
| Young’s modulus $E$, 1000°C [GPa] | 81.7      | 81.7   |
| density $\rho$ [kg/m³]      | $7.1 \times 10^3$ | $7.1 \times 10^3$ |
| creep activation energy $Q$ [kJ/mol] | 486       | 452    |
| creep exponent $n$ [-]       | 5.29      | 41.0   |
| creep prefactor $A_0$ [MPa$^{-n}$s$^{-1}$] | $1.72 \times 10^{-10}$ | $3.46 \times 10^{-124}$ |
| creep factor $a$ [K$^{-1}$]  | -0.012    | 0.10   |

Table 1. Material parameters of Fecralloy and MA956.

Creep was permitted in all layers (slow creep parameters for TGO and TBC from [2]). The creep rate in the TBC and in the TGO was calculated with a Norton creep law $\dot{\varepsilon} = A\sigma^n$. The creep rate of Fecralloy and MA956 is calculated by

$$\dot{\varepsilon} = A_0 \cdot \exp(aT) \cdot \exp\left(-\frac{Q}{RT}\right) \sigma^n$$

with the activation energy $Q$, the creep exponent $n$ and an additional factor $a$ (Tab. 1). The creep parameters $Q$, $A_0$, $n$, and $a$ are fitted values obtained from experimental creep tests. The resulting maximum growth stresses inside the TGO are in the range of 0.1 to 1 GPa and are of the same order of magnitude as shown in [6].

The TGO growth was simulated by simplifying the process as isotropic swelling. A Tammann law was used to describe the oxidation [7, p. 268]:

$$\dot{s} = \frac{1}{2} \cdot \frac{k_p^v}{s^2}$$

with the current TGO thickness $s$, the parabolic oxidation constant $k_p^v$ and the growth rate $\dot{s}$. The parabolic oxidation constant of this simulation is $k_p^v = 1.5 \times 10^{-17}$ m²/s which describes the oxidation kinetics of $\alpha$-$\text{Al}_2\text{O}_3$ at 1000°C [4]. The growth rate was calculated once at the beginning of the simulation and is constant for the further simulation.
Figure 2. Growth stresses of the TGO at 1000°C (hold time 2 h) in the Fecralloy and MA956 coating system against the initial TGO thickness.

3. Results

Fig. 2 shows the radial stress $\sigma_{11}$ at the substrate/TGO and the TGO/TBC interfaces against the respective initial TGO thickness. The radial stresses decrease while increasing the initial TGO thickness because the growth rate of the TGO decreases while increasing the TGO thickness (Eq. 2). The TGO growth is governed by oxygen diffusion through the TGO [4]. The stresses in the MA956 substrate are greater than the stresses in the Fecralloy substrate for all TGO thicknesses. This relation changes in the TBC: The TBC stresses in the Fecralloy coating system are larger then the TBC stresses in the MA956 coating system.

Fig. 3 shows the distribution of radial stress after 2 h at 1000°C in Fecralloy and MA956. The reason for the stress maximum inside the MA956 substrate was discussed in [4]. The growth of the TGO in lateral direction results in compressive stresses in the peak and tensile stresses in the valley of the TBC. Furthermore, it results in a changed position of the TGO in which the valley of the TGO is shifted to the inside (in Fig. 3 to the left) and the peak to the outside (in Fig. 3 to the right). The comparatively fast creeping Fecralloy substrate can not resist the strain because of the resulting low stresses. The resistance of the MA956 substrate to the strain of the TGO is larger caused by the creep strength. This leads to higher magnitude of stresses inside the substrate and to lower stresses inside the TBC. Thus, it can be expected that the Fecralloy coating system fails most likely inside the TBC and MA956 coating systems inside the substrate or at the interface substrate/TGO.

The prediction of different failure mechanisms of the studied substrate materials was validated with experimental tests. Fig. 4(a) shows a micrograph of a Fecralloy sample with a cyclic grown TGO (no applied initial TGO). The crack path of the coating system is above the TGO inside the TBC layer. Fig. 4(b) shows the failure of the ODS strengthened MA956 sample, also with a cyclic grown TGO. The failure occurs at the TGO/substrate interface, which correlates with the distribution of stresses in Fig. 2. For this reason, the creep strength of the used substrate has a large influence on the position where the failure is induced and the resulting crack path, even if adequate MCrAlY materials are used as a bond-coat layer in technical thermal barrier coating systems.

The simulation of the growth stress shows that slow creeping substrates and bond-coats respectively reduce the lifetime caused by cracks under the TGO. On the other hand a more creep strengthened bond-coat reduces the stresses inside the TBC. MA956 samples with an artificial applied initial TGO by preoxidation or sputtering fail more likely under the TGO.
σ_{11} stresses in the Fecralloy model. 

σ_{11} stresses in the MA956 model.

Figure 3. Growth stresses of the TGO at 1000°C (hold time: 2 h, initial TGO thickness: 2 μm).

Figure 4. Comparison of the failure in coating systems with Fecralloy and MA956 substrates (~300 cycles, 2 h at 1050°C each).

Fecralloy samples with an initial TGO fail only above the TGO. This suggests that there is an optimum of the bond-coat creep strength. These results contradict the considerations from Padture et al. [1] and Evans et al. [8]. They discuss that only slow creeping bond-coat materials benefit the lifetime of the coating systems.

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