HEALING PARTICLES IN SELF-HEALING THERMAL BARRIER COATINGS

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Keywords: selective oxidation, encapsulation, ceramic coatings, fracture mechanics, thermal stress, finite element simulations

ABSTRACT

Crack healing in ceramic thermal barrier coatings (TBCs) may be realized by embedding Mo-Si based particles in the thermal barrier coating. Upon cracking, these particles are exposed to oxygen that permeates through the top layer and the crack gap is filled with SiO_2 which is produced from oxidation at high temperature. Due to its amorphous characteristics and expanding oxide volume, SiO_2 is able to fill a significant portion of the crack. Simultaneously, Mo forms a volatile oxide (MoO_3) that may leave the coating through the crack path and subsequently through pores, thereby compensating for the volume increase upon oxidation. The present work combines an experimental and modelling approach to develop and characterize the healing particles in the TBC system. In particular, two issues have been addressed, namely (i) the manufacturing of the healing particles that are to be embedded in the coating and (ii) the characterization of damage in TBC systems in order to identify the optimal properties of the healing particles.

1. INTRODUCTION

Thermal barrier coatings (TBC) deposited by air plasma spraying onto hot components in gas turbine engines ultimately fail by the development of cracks that cause delamination [1,2]. These cracks nucleate and grow upon thermal cycling due to thermal stresses that originate from the mismatch in thermal expansion coefficients of the distinct layers that compose the TBC system. Healing of these cracks during service will extend the lifetime of the engine components and reduce maintenance costs.

The healing particles can be encapsulated to prevent premature formation of SiO_2 during operation. Selective oxidation of $Mo(Si_{1-x}Al_x)_2$, prior to embedding the particles, may be an easy and cost-effective method to realize the desired encapsulation. Next, knowledge of the damage mechanisms in TBCs is essential in order to design a particle-based healing system. In particular, it is important to embed healing particles in regions where cracks are likely to initiate. Furthermore, the size and number of healing particles in these critical regions must be optimized with the purpose of developing an efficient and robust self-healing system.

2. MATERIALS AND METHODS

Oxidation of $Mo(Si_{1-x}Al_x)_2$ healing particles may generate particles consisting of a shell of alumina (α-Al_2O_3) with a core of Mo-Si. Since Al has a very high affinity to oxygen, it tends to oxidize first amongst Mo and Si. For the application, on hand design of these particles is prerequisite. The thickness of the alumina shell δ depends on the size d and composition x of the original spherical particle considering that all Al is consumed by selective oxidation according to:

$$\delta = d\left(\left(1+\frac{xM_s\rho_p}{M_p\rho_s}\right)^{1/3} - 1\right),$$

where M_p and M_s denote the molecular weights, ρ_p and ρ_s the densities of the particle and the shell, respectively.

In order to understand the failure mechanisms under thermal loading, three-dimensional finite element analyses (FEA) have been carried out on macroscopic specimen and microscopic Representative Volume Elements (RVEs) of a TBC. The effect of the substrate on the microscopic RVE is taken into account through macroscopic displacements imposed as boundary conditions at the microscale. These displacements are obtained from the macroscopic analysis, where a finite element model of a macroscopic specimen is employed with two layers, one representing the homogenized TBC and the other representing the substrate as shown in Figure 1a.

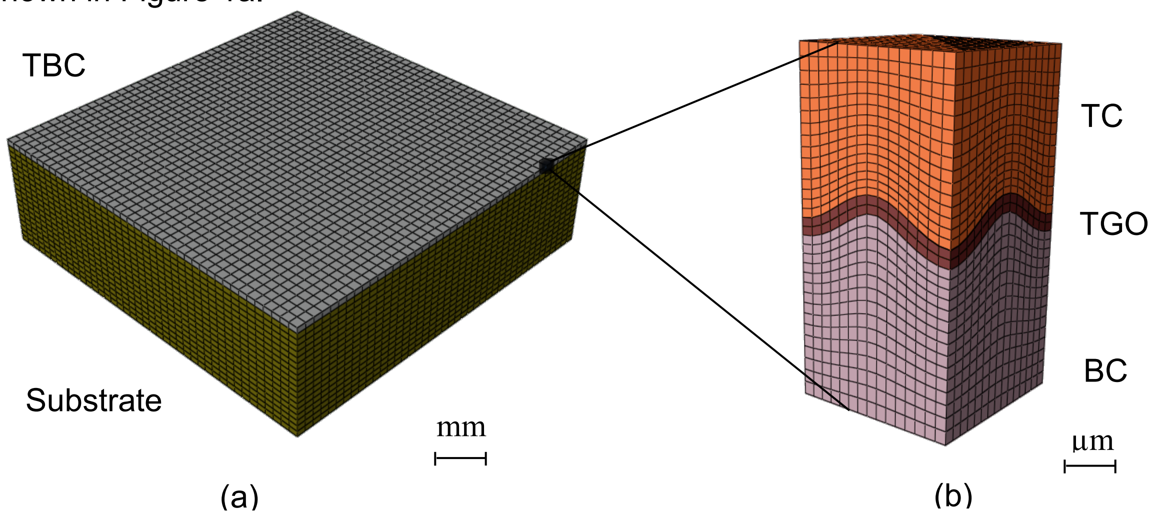

Figure 1: Finite element model of TBC system representing the Bond Coat (BC), Thermally Grown Oxide (TGO) and the Top Coat (TC): (a) coated substrate (macroscale), (b) volume element in TBC (microscale)

The microscopic finite element model of the TBC system is shown in Figure 1b. The RVE consists of three layers of the TBC system representing the Bond Coat (BC), Thermally Grown Oxide (TGO) and the Top Coat (TC). In this study, the interfaces between the layers (TC/TGO and TGO/BC) are modelled as a double-sinusoidal surface. Interface irregularities are known to be one of the key drivers for crack initiation in this inhomogeneous system [2] since they allow large in-plane compressive stresses (generated during cooling) to eventually produce out-of-plane tensile stresses.

3. RESULTS AND DISCUSSION

The explicit relation between the alumina shell thickness δ and the diameter d of the healing particle is displayed in Figure 2 for different fractions x of Al.

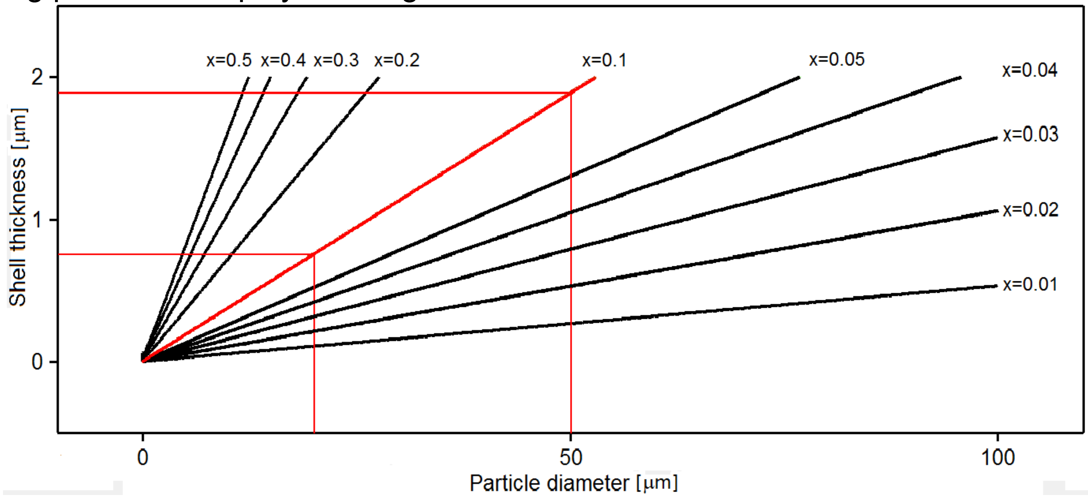

Figure 2: Relationship between the alumina shell thickness and the size of $Mo(Si_{1-x},Al_x)_2$ spherical healing particle for different compositions.

When applying a TBC with plasma spraying, the size of the healing particle should be within 20 to 50 µm due to manufacturing constraints. Correspondingly, if the Al fraction x equals 0.1, then the thickness of the alumina shell will be in the range of 0.8 and1.9 µm; cf. Figure 2.

In order to simulate the fracture in the TBC, cohesive elements at the microscale are being used. Both macro and micro specimens are subjected to the same thermal load consisting of a temperature change of 1000 °C. The FEA results corresponding to RVEs near the edge and the middle of the macroscopic specimen coated with a TBC are shown in Figure 3. Red color indicates the regions that are cracked, whereas the blue colored portions are intact.

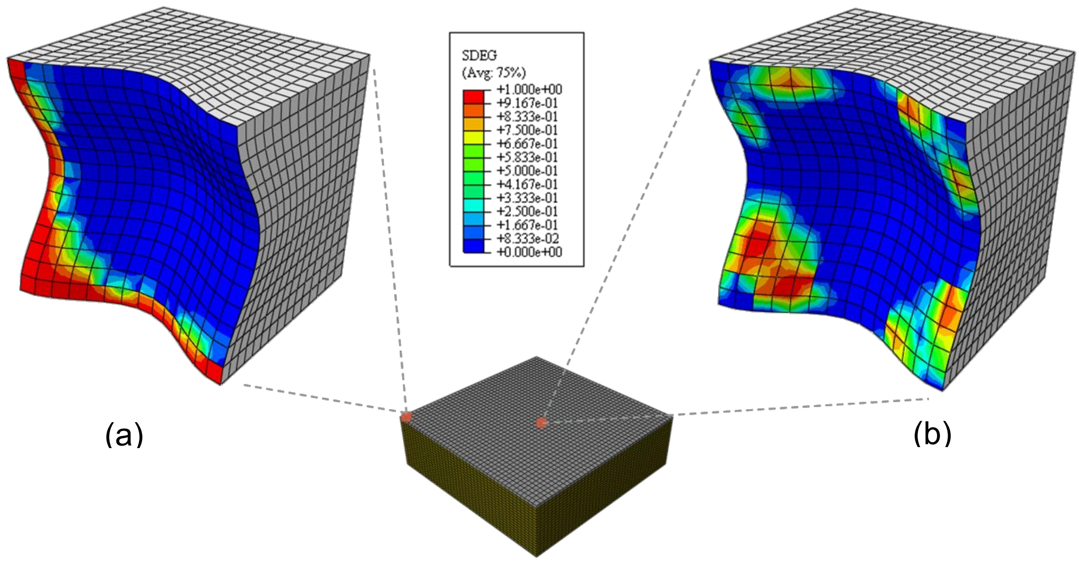

Figure 3: Typical crack pattern in TC/TGO interface of an RVE (a) near the edge of specimen, (b) in the interior of specimen

For points near the edge of the macroscopic specimen, delamination cracks initiate at the free edge as may be observed in Figure 3a. On the other hand, for the RVE in the interior of the macroscopic specimen, cracks initiate at valleys of the TC/TGO interface as shown in Figure 3b. This study will help to identify the critical regions where the healing particles can be embedded.

4. CONCLUSION

Encapsulated Mo-Si healing particles with an α-Al_2O_3 shell of about 1 µm embedded in matrix of a TBC prepared by plasma spraying may be realized by selective oxidation of $Mo(Si_{1-x}Al_x)_2$ with x of 0.1.
The finite element simulations of the crack damage in a TBC system due to thermal loading indicate that the healing particles should be placed preferentially close to the TC/TGO interface particularly, if the surface roughness is large.

ACKNOWLEDGEMENTS

Financial support from the Netherlands Innovation Oriented Program (IOP) on Self Healing Materials, grant number SHM01021, is gratefully acknowledged.

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