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Modelling the fracture behaviour of thermal barrier coatings containing healing particles

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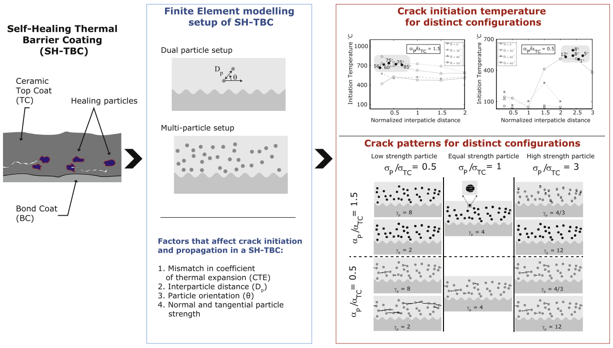
HIGHLIGHTS

- Mismatch of thermomechanical properties strongly affects effectiveness of particle-based self-healing thermal barrier coating
- High ($\geq$1.5) or low ($\leq$0.5) mismatch in coefficient of thermal expansion is generally detrimental due to premature cracking
- Successful self-healing TBC design may be achieved with healing particles that have a slightly low CTE and fracture strength
- Crack pattern for high (resp low) CTE mismatch is controlled by Mode I (resp II) adhesion strength of particles in top coat
- Predictions on the critical cracking temperature cannot be based on volume fraction only

GRAPHICAL ABSTRACT



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ABSTRACT

The performance of a self-healing Thermal Barrier Coating (TBC) containing dispersed healing particles depends crucially on the mismatch in thermomechanical properties between the healing particles and the TBC matrix. The present work systematically investigates this phenomenon based on numerical simulations using cohesive element-based finite element analysis. The effect of the mismatch in Coefficient of Thermal Expansion (CTE) and fracture strength between the healing particles and the matrix on the fracture characteristics is quantified in detail. Unit cell-based analyses are conducted on a representative self-healing TBC system under a thermal loading step typically experienced by TBC systems in jet turbines. Two different simulation setups are considered within the TBC unit cell namely (i) a single pair of healing particles and (ii) a randomly distributed array of healing particles. The results of the simulations are reported in terms of the fracture pattern, crack initiation temperature and crack length for various CTE mismatch ratios. Correlations are established between the results obtained from the two simulation setups essentially revealing the effect of spatial distribution and proximity of healing particles on the fracture pattern. The results obtained from the analyses can be utilised to achieve a robust design of a self-healing TBC system.

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1. Introduction

Thermal Barrier Coating (TBC) systems are protective layers applied to critical structural components of jet engines operating at high-temperature. A typical TBC system consists of three different layers, (i) a Top Coat (TC), which directly faces the hot gases in the engine,(ii) a Thermally Grown Oxide layer (TGO) and (iii) a Bond Coat (BC) layer which is connected to the actual turbine blades. The TC layer is a ceramic layer usually consisting of Yttria Stabilized Zirconia (YSZ). It provides thermal insulation to the underlying components because of its low thermal conductivity. The BC layer is an intermediate metallic layer often made of NiCoCrAlY alloy. It acts as a bonding layer connecting the TC and the substrate and also provides oxidation resistance to the substrate by acting as a sacrificial layer. The TGO layer is a relatively thin α alumina (Al_2O_3) layer formed due to the oxidation of the aluminium phase in the BC at high temperatures. The coating system undergoes a thermal cycle during each start and stops as the turbine's temperature increases from ambient to operating temperature and subsequently decreases back to the ambient temperature. During each thermal cycle, the layers of the TBC system expand and shrink unequally due to a mismatch in coefficients of thermal expansion (CTE) of the TBC layers as illustrated in Fig. 1a. The resulting thermal stresses cause nucleation and growth of micro-cracks in the TBC system [1,2]. In addition, cracking also occurs due to the thickening of the TGO layer as the oxidation of the metallic bond coating generates more alumina, see Fig. 1a and b. After several hundreds of thermal cycles, the micro-cracks eventually coalesce, forming a relatively large crack originally more or less parallel to the TBC-substrate interface. As large cracks deflect towards the free surface via local imperfections, the TBC separates from the substrate, which is known as spallation, as illustrated in Fig. 1b. As a consequence, large portions of the TC separate, which may lead to direct exposure of the critical engine components to the high-temperature gases, ultimately resulting in a catastrophic failure of the entire turbine.

Several efforts have been made to increase the lifetime of the TBC system, mainly in the directions of varying the deposition process and coating compositions in order to delay the initiation of micro-cracks [3-5]. Incorporating self-healing mechanisms in TBC systems is a novel approach to improve the lifetime of these coatings [6-10]. The principle of the self-healing mechanism in a TBC system is demonstrated in Fig. 1c [7]. A solid self-healing agent is encapsulated and embedded within the TBC topcoat layer during the coating process. When the crack induced by thermal cycling reaches the microcapsule, the capsule breaks and the oxidised self-healing agent flows into the crack, where it can further react with the matrix material and heal the crack. The best studied concept of the self-healing TBC is based on alumina coated Mo-Si particles embedded in the TC layer close to the TC/BC coat interface where the micro-cracks are likely to initiate. Upon cracking in the TBC, the micro-cracks interact with the healing particles, resulting in fracture of the particles. Subsequently, the healing agent within the particles oxidises and diffuses into the crack to form a glassy phase which in turn reacts with the surrounding matrix to form a load-bearing crystalline ceramic (zircon). The resulting healing of the micro-cracks delays the formation of a macro-crack by preventing crack coalescence which, in turn, extends the life time of the TBC system. Further details of the above-discussed self-healing TBC system such as detailed description of the healing mechanism, type of healing particle, fabrication routes and associated challenges can be found in the following works [6-8, 11-13].

Numerous computational studies have been conducted to investigate the failure mechanisms in the TBC system. In the context of fracture analysis in TBC systems, different approaches have been used, including, classical fracture mechanics-based methods (e.g. VCCT, energy release rate) [14,15], cohesive zone element based methods [16,17] and the extended finite element method (XFEM) [18,19]. Classical fracture mechanics approaches are suitable for crack propagation studies, whereas cohesive element-based approach enables modelling of crack initiation as well as crack propagation. XFEM is an enriched version of the classical finite element method which embeds discontinuities in the shape functions of a classical 2-D or 3-D finite element. This method serves as a tool to represent initial and evolving crack geometry independent of the finite element mesh and the crack evolution can be modelled either using classical fracture mechanics parameters or cohesive traction-separation laws. One of the current shortcomings of XFEM is its limited capability in dealing with multiple cracking and coalescence, which are crucial in the current study. Cohesive elements were utilised successfully for such multiple cracking and coalescence problems albeit with higher computational costs to achieve 'mesh-independent' solutions. A detailed review on various modelling methodologies and failure mechanisms in TBC systems addressed through computational modelling can be found in [20]. A second review on the influence of modelling choices in terms of interface morphology, boundary conditions, dimensionality and material models on the TBC response is presented in [21]. They provided guidelines and strategies for effectively modelling the stress evolution and the crack propagation in TBC systems. All

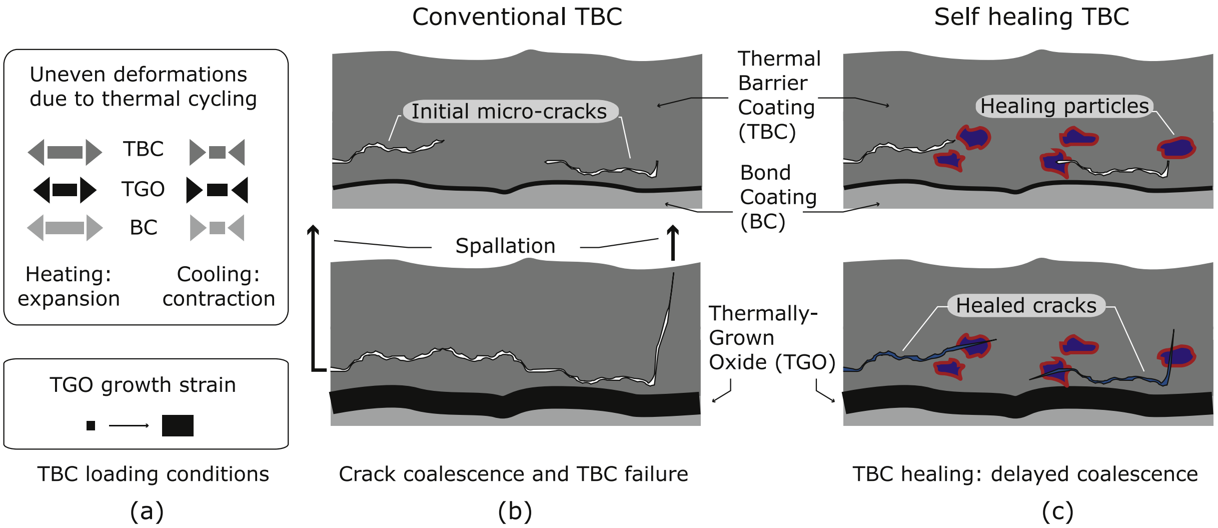

Fig. 1. Schematic of TBC failure mechanisms and principle of a self-healing TBC system.