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# Tailoring of self-healing thermal barrier coatings via finite element method

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ABSTRACT

In this paper, the multi-layer structured self-healing thermal barrier coatings (TBCs) have been designed and optimized on the basis of design criteria of the typical double layer NiCrAlY/YSZ TBCs. The self-healing layer 20%wt.TiC + $x$Al$_2$O$_3$ + (80 wt.%-$x$) YSZ (TAZ) has been embedded between the NiCrAlY and YSZ layer. Based on the better thermal insulation and remission of thermal expansion misfit, the optimized $x$ and the thickness ratio of each layer for the designed self-healing TBCs has been obtained. And the self-healing effect of the TBCs under high temperature service condition was also simulated. The detailed self-healing mechanism has been discussed systematically. The investigation results indicate that there are three factors which will promote the self-healing effect of the designed multi-layer structured self-healing TBCs, i.e. the larger compressive stress induced around the crack, the filling of the self-healing matter in the crack and the reduction of formation rate of the TGO layer. In addition, the existence of self-healing cracks which are near to the interface will also change the stress distribution along the top-coat/self-healing layer interface evidently.



## 1. Introduction

Thermal barrier coatings (TBCs) which are often coated onto the superalloy substrates are very important structural and functional coatings. It was widely used in many hot-section industrial components, such as aero-engine combustor and turbine blade [1–6]. Although the TBCs can be fabricated by different processing techniques, the failure is inevitable when the TBCs were endured with high temperature oxidation, corrosion, thermal shock, foreign object damage (FOD) etc. The initiation, nucleation and propagation of the cracks in the TBCs accelerate the failure of the TBCs [7–11]. How to control the degradation process of the TBCs is very important. The reliability and durability are the two key aspects for the usage of the TBCs. The reliability usually demand that the TBCs has high adhesive strength, enough thermal insulation effect and thermal shock resistance. The durability usually demands that the TBCs has long lifespan during high temperature service. The reliability is the basis for the usage of the TBCs, and the durability is the demand for the application of the TBCs. As for both aspects, the TBCs must have a certain ability to resist the crack propagation.

Whatever the failure modes are, the intrinsic reason which cause the TBCs failure is the crack initiation and propagation. The modes of the crack propagation are usually very different for the TBCs fabricated with different processing techniques. Even the TBCs are fabricated by the same processing techniques, the failure patterns are also different when they were endured with different service conditions [12–15]. As for the TBCs fabricated by atmospheric plasma spraying (APS), the coating usually exhibits lamellar and porous structure, cracks tend to initiate at the inner of the ceramic layer or at the interfaces. As for the TBCs fabricated by electron beam-physical vapour deposition (EB-PVD), the TBCs usually presents the columnar structural characteristics from the cross-section view, while the surface shows pebble shape structural characteristics. The interface between the top-coat and bond-coat usually has high adhesive strength, the failure is mainly attributed to the fracture of the single columnar grains, cracks may propagate along the interface among the adjacent columnar grains, and the existed gap between the adjacent columnar grains will dispatch the propagation energy of the cracks [16,17]. As for the TBCs fabricated by PS-PVD technique, the TBCs usually exhibits columnar structural characteristics from the cross-section view, but the displacement between the adjacent columnar grain is more dense compared with that of the EB-PVD TBCs, the surface of this type of

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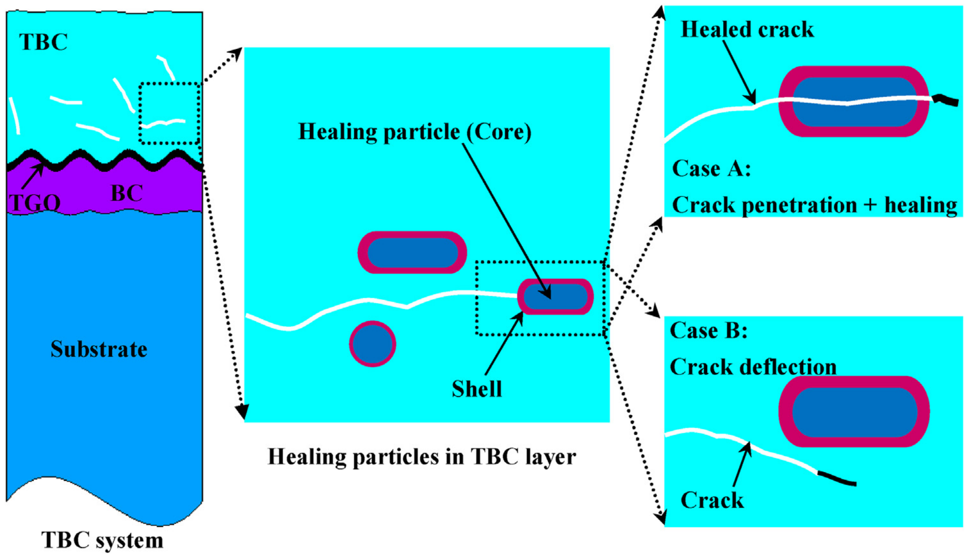


**Fig. 1.** Schematic illustration of the self-healing mechanism of the TBCs at high temperature.

TBCs usually shows the cauliflower-like structural characteristic. The failure modes also exhibit the spalling of the parts of columnar grains, cracks can hardly propagate along the interfaces among the columnar grains due to the large gap between the adjacent columnar grains [18–21].

But once the TBCs fabricated by EB-PVD or PS-PVD were endured with foreign object damage (FOD) or impact corrosion, the cracks may initiate and propagate in the columnar grains. The EB-PVD TBCs and PS-PVD TBCs usually have high thermal shock resistance compared with that of the APS-TBCs due to the high stain tolerance, but they usually has higher thermal conductivity compared with the APS-TBCs which is attributed to that the gap between the adjacent columnar grains are usually parallel to the heat flux direction (through-thickness direction). While in the APS-TBCs, cracks play an important role in controlling the thermal shock resistance or effective thermal conductivity, the quick propagation of the cracks will accelerate the failure of the TBCs [22].

Self-healing TBCs usually has specific functionality. When a crack begins to propagate, the stress concentration will appear at the crack tip, once the stress become large compressive stress when the crack propagate, the closure of crack will happen. From another aspect, when some materials has been released in the TBCs and fill the gap of the crack, the crack will be also sealed. In addition, if the stress field around the crack is compressive stress, this will also promote the closure of the crack. All these cases can be called self-healing effect. Many literatures have reported the self-healing effect of the bulk-ceramic and coating from the experimental investigation aspects [23–26]. As for the TBCs, W.G. Sloof et al. [27] have described the possible self-healing mechanism for the TBCs when they were endured with high temperature. The basic process of self-healing is illustrated depicted in Fig. 1. When the TBCs were suffered with thermal stress or other exterior loads, micro-cracks can produce at the inner or the interface of the TBCs, when the micro-crack propagate to the zone where is near to the 'capsule', the 'capsule' will broke and will release some self-healing substances (usually are metal or alloy materials), the substances will fill the crack, and the crack could not continue to propagate (Case A). If the micro-cracks bypass the 'capsule', the self-healing will not happen (Case B). To produce the case A rather than B is a direct path to realize the self-healing process of the TBCs at high temperature.

The self-healing bulk ceramic or composites usually has the same characteristics, i.e. the glassy state substances at high temperature can be formed, and this type of substance can fill the gap of the crack and inhibit the crack to propagate and thus improve the fracture toughness and prolong the service life of the ceramics [28–32]. Micromechanical modelling with the aid of the Eshelby-Mura equivalent inclusion method can be used to study various aspects of the complex three-dimensional interaction between a crack and a microcapsule in the self-healing composites. The stress distribution around the cracks, the microcapsules or at the crack tip can be obtained in order to understand the self-healing mechanism of the self-healing composites [33,34]. In fact, many cracks are disastrous for the TBCs when they were endured with external load. Once the TBCs have a certain self-healing ability, the crack propagation will be delayed or stopped, the lifespan of the TBCs under high temperature service conditions will be extended. Especially, as for the APS-TBCs, the propagation of the cracks at the inner of the ceramic layer of the TBCs or around the top-coat (TC)/thermally grown oxide (TGO) interface will be controlled by many exterior factors besides the intrinsic microstructural characteristics of the TBCs. Such as the service temperature, temperature gradient, exterior oxidizing gas, exterior mechanical load [35–38]. The generation of the self-healing effect will delay the dynamic progress of the propagation of the crack, and thus delay the eventual failure of the TBCs.

In this paper, the multi-layer structured self-healing TBCs were tailored via finite element modelling, the structure and composition of the TBCs with self-healing effect has been designed and optimized. And the self-healing effect of the tailored TBCs has also been simulated. Especially, the detailed self-healing mechanism for the designed and optimized TBCs has been discussed systematically. Some interesting results have been presented, and the simulation results will provide a design criteria for the self-healing TBCs with excellent performance.

## 2. Simulation procedures

### 2.1. Design criteria

In the current work, the multi-layer structured self-healing TBCs have been designed and optimized according to the design criteria of the typical double layer NiCoCrAlY/YSZ TBCs based on the previous experimental work [39]. The self-healing layer 20%wt.TiC + $x$Al$_2$O$_3$ + (80 wt.%-$x$)YSZ (TAZ) has been embedded between the NiCoCrAlY and YSZ layer (Fig. 2). The intent of the addition of Al$_2$O$_3$ is to improve the barrier effect of exterior oxy-