

## Effect of pre-existing microcrack on the cyclic displacement instability in thermal barrier coating systems

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**Abstract** The displacement instability of the thermally grown oxide (TGO) layer in thermal barrier coating systems is a critical factor inducing the failure of the system by causing large scale delamination and spallation. In this paper, the effect of pre-existing microcracks within the ceramic top-coat (TC) on the cyclic displacement instability under thermal cycling is investigated by a finite element analysis. Stress and the interface morphology are obtained after thermal cycling when the microcracks pre-exist within the TC. The influence of various parameters including crack location, crack length and crack direction on the interface morphology are discussed in detail. It is demonstrated that the existing of microcracks within TC can aggravate the displacement instability and affect the stress state in TC significantly. However, when the crack is perpendicular to the flat interface, the aggravation of it on the instability is weakest.

**Keywords** Microcracks, Displacement instability, Thermal cycling, Thermal barrier coating

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### 1. Introduction

Thermal barrier coating (TBC) system is widely used in the blades of gas turbines or aircraft engines as the thermal insulation component, which can protect the base material against the extreme temperature due to its low heat conductivity. Usually, a typical TBC system consists of the following multilayer (Fig. 1a): (i) a thick superalloy substrate, (ii) a bond-coat (BC) next to the substrate protecting the substrate from oxidation, (iii) a ceramic top-coat (TC) for providing thermal insulation, and (iv) a thermally grown oxide (TGO) layer forming between TC and BC due to the high temperature oxidation[1-4].

The durability of TBC focuses world attentions in recent years. The coating performance usually begins to degrade associated with the large scale delamination and spallation of TC. Studies have confirmed that the displacement instability of TGO (Fig. 1) under cyclic oxidation is a critical factor inducing the fracture and delamination in TBC made by electron beam-physical vapor deposition (EB-PVD) [2, 5-9]. The most vivid manifestation of the instability is the downward displacement of TGO into soft BC (Fig. 1a), which is motivated by the large residual compressive stress caused by thermal expansion misfit and the thermal growth of TGO [6, 10, 11]. The instability usually initiates at the region near the imperfection of BC-TGO interface and the amplitude of it extends as the extensive thermal cycling. Following factors have confirmed to have a strong influence on the instability [2, 3, 5, 6, 12-19]. (i) The thermal cycling: It is a necessary condition to cause large instability; (ii) The growth strain resulting from the volume increase in the process of BC transforming to new TGO by high temperature oxidation; (iii) The initial morphology imperfection in the BC-TGO interface; (iv) The accumulation of plastic strain in BC near the initial imperfection, which is the most relevant factor controlling the evolution of displacement instability, and (v) The creep behavior of component materials.

Due to the need of enhancing the strain tolerance of the ceramic coating, the microcracks are widely introduced in the process of coating deposition [20, 21]. Many experimental and analytical results have confirmed that pre-existing vertical surface cracks in TC can enhance the resistance to the initiation of interface crack [22-26]. Therefore, when these cracks exist at the surface of the TC, they can provide an additional capability to prevent the interface cracks developing besides enhancing the coating strain tolerance. However, as shown in Fig. 1a, these introduced microcracks

also widely exist within the TC. Experimental investigations have shown that when these microcracks appear in the region near the site of displacement instability, they would nucleate and extend as thermal cycling under the large tensile stress [5], and finally cause large scale delamination and spallation at the interface of TC-TGO [3, 4]. Based on Mumm's experiment results, Karlsson [14] modeled these cracks as traction-free internal planes and found that these cracks also can significantly promote the extending of the instability. Therefore, the existing of microcracks near the instability site would affect the durability of the system. Similarly to the surface cracks, there would be an optimal direction for the internal cracks, in which the effect of these cracks on the instability extending is weakest.

However, in all of the previous studies focusing on the displacement instability, the effect of the geometric parameters of pre-existing cracks within the TC on the instability was not considered [2, 5-7, 13-15, 19, 27] and the optimal direction is still not obtained. Hence, the objective of this paper is to explore the effect of pre-existing cracks within TC of varying length, location and direction on the displacement instability of TGO under thermal cycling and try to obtain the optimal crack direction, in which the instability development is weakest. The results may be helpful in controlling the instability and providing the probability to design a longer life TBC.

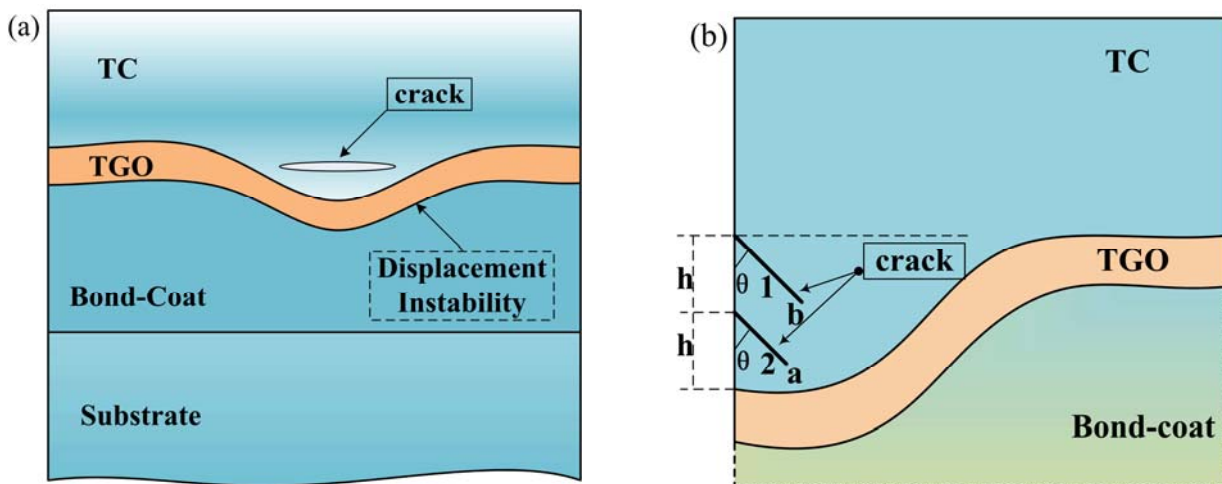


Figure 1. Schematic for (a) the multi-layer TBC system with TGO displacement instability, and (b) the microcracks within TC above the instability site.

## 2. Statement of the problem

Due to the microcracks appearing in the region near the site of TGO displacement instability can significantly promote the extending of instability and induce the final failure of TBC system, we only consider the case where the initial crack exists above the instability site in this problem. As shown in Fig. 1b, two different cracks are introduced in this problem: crack “a”, which is at a distance  $h$  away from the base of instability region extending from the symmetry axis to the inward of TC, and crack “b”, which is at a distance  $2h$  from the base with the same morphology as crack a. Each of these two cracks is defined by the included angle  $\theta_1$  and  $\theta_2$  (Fig. 1b), respectively. It must be noted that these two cracks are not considered in this problem together and only a single static crack problem is solved. In this problem, all materials are assumed to be isotropic (the detailed material properties are described below) and the plane strain condition exists. In order to investigate the extending of instability zone under thermal cycling when the crack exists above the instability site, cyclic thermal load is applied. In each thermal cycle, the system is cooled to ambient temperature from an initial peak temperature firstly and a thermal stress analysis is carried out associated with this temperature change. Then, the temperature rises to the initial state

with a new stress state being obtained, and this peak temperature would hold a long time, where the thermal growth of TGO layer would occur. After that, the system is cooled to ambient again. The cyclic thermal load is obtained by repeating this sequence many times.

### 3. The simulation scheme

#### 3.1. Description of model

Due to the complexity of the morphology of interface and crack, the finite element method (FEM) is used to solve the problem. A conventional FEM model for the displacement instability is adapted in the calculations (Fig. 2) [13, 14]. The analysis is carried out by employing the computer program ABAQUS with the four-node, bi-linear plane strain elements. Geometric dimension of each layer is shown in the model and an initial instability zone with a depth  $2h = 7.5\mu\text{m}$  and radii of curvature  $R_1 = R_2 = 11.25\mu\text{m}$  is introduced. All the nodes at the right sides of the model are allowed to move with a limit of keeping an equal displacement in the X direction for them and a symmetric boundary condition is applied to the left side. The nodes on the bottom side are fixed in the Y direction to avoid rigid body motion.

In the analysis, the initial static crack is not allowed to propagate, and the length  $L$  and the angle  $\theta$  for both cracks are changed as variables. The crack behavior is achieved by using the extended finite element method (XFEM) [28-31], which can simulate the crack behavior without the crack tip conforming to any node point of the finite element mesh. In addition, in all calculations, only the case of single crack within the TC is simulated and the case of multi-crack is not considered in this paper.

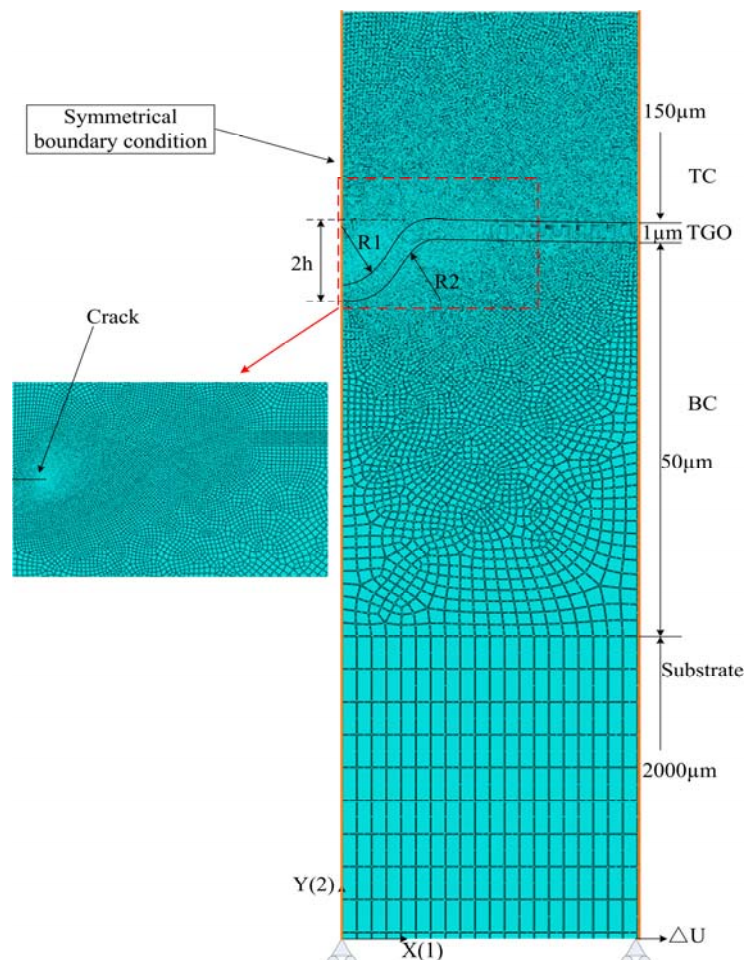


Figure 2. Finite element method model for the crack within the TC above the instability site.

### 3.2. Material properties

All materials used in the calculations are assumed to be isotropic and all material properties are temperature-dependent, which are summarized in [32]. Both TC and substrate are linear elastic and BC is considered as elastic-perfectly plastic with a temperature-dependent yield strength. The user subroutine, *uexpan*, in ABAQUS is employed to simulate the thermal growth of TGO, which was introduced by Karlsson and Evans in [13]. The growth behavior is achieved by imposing a thermal strain at the holding time of high temperature. The thermal strain consists of two components:  $\varepsilon_g$ , which is a lateral growth strain parallel to the TGO-BC interface, and  $\varepsilon_t$ , which is a thickening strain. In this paper, a ratio of lateral growth strain to thickening strain,  $\varepsilon_g / \varepsilon_t = 0.5$ , is used with  $\varepsilon_g = 1 \times 10^{-3}$ . Also, the TGO is allowed to yield at the peak temperature with a yield strength  $\sigma_Y^{tgo} = 1$  GPa and it is elastic in other temperature [13]. The sequence of thermal load is repeated 24 times with 3 hours hold time at peak temperature (1100°C) for each sequence [6, 13, 14].

## 4. Results and discussions

### 4.1. General response

Initial results are generated for an intact TC, a TC within a crack at location “a” and a TC within a crack at location “b” (Fig. 1b), respectively. Cracks in both cases have an initial length,  $L = 4 \mu\text{m}$  and  $\theta_1 = \theta_2 = 90^\circ$  in this section. A synopsis of the major findings is presented in Figs. 3-5.

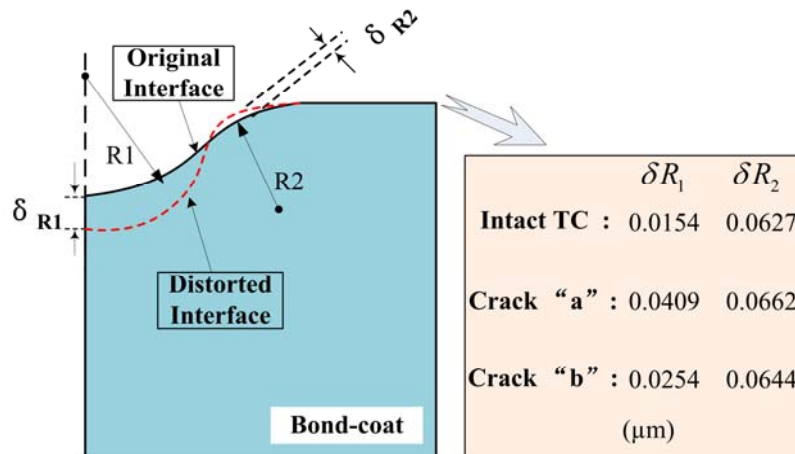


Figure 3. The distortions of BC interface after 24 thermal cycles.

Fig. 3 shows the morphology of BC-TGO interface after 24 thermal cycles. It can be seen that the interface is distorted significantly with large upward displacements around the periphery of the instability zone and large downward displacements at the base. This phenomenon is in accordance with the previous results found by experiments and simulations [5, 6]. The shape distortions at the interface are induced by the plastic deformation in BC directly, and thermal misfit stresses and thermal growth stresses are two main resources to cause the plastic deformation. From Fig. 3, we can see that all these distortions at BC-TGO interface can be represented by the change of  $R_1$  ( $\delta R_1$ ) and  $R_2$  ( $\delta R_2$ ). Therefore, in following discussions, we mainly focus on the parameters  $\delta R_1$  and  $\delta R_2$ . Fig. 3 also presents the change of  $R_1$  ( $\delta R_1$ ) and  $R_2$  ( $\delta R_2$ ) when an initial crack exists within TC. It clearly shows that the distortion of the interface is more significant when the microcrack exists within TC, especially the downward displacement  $\delta R_1$ . In addition, the crack location also

can affect the interface distortions. Compared to the crack “b”, the crack “a”, which is more close to the base of the instability zone, results in a more significant distortion. Therefore, the existing of crack, especially the crack close to the base of instability site, can induce larger "up" and "down" displacements.

The distribution of out-of-plane stress ( $\sigma_{22}$ ) in the intact TC presents in Fig. 4b. The tensile stresses mainly concentrate on the region above the instability site. When the tensile stress develop to a sufficient level, it can induce the cracks within the TC above the instability site and the delamination at the interface[5, 16]. The compressive stresses mainly appear in a relatively small zone near the periphery of instability zone and this compressed zone can prevent the crack initiation. Fig. 5A demonstrates the distribution of out-of-plane stress in TC along TC-TGO interface when a crack exists within TC. It can be seen clearly that the tensile stress level near the instability region would increase when the crack exists at location “a” and this increase recedes when the crack is far away from the instability region (location “b”). In other regions, the effect of crack on  $\sigma_{22}$  is small and can be ignored.

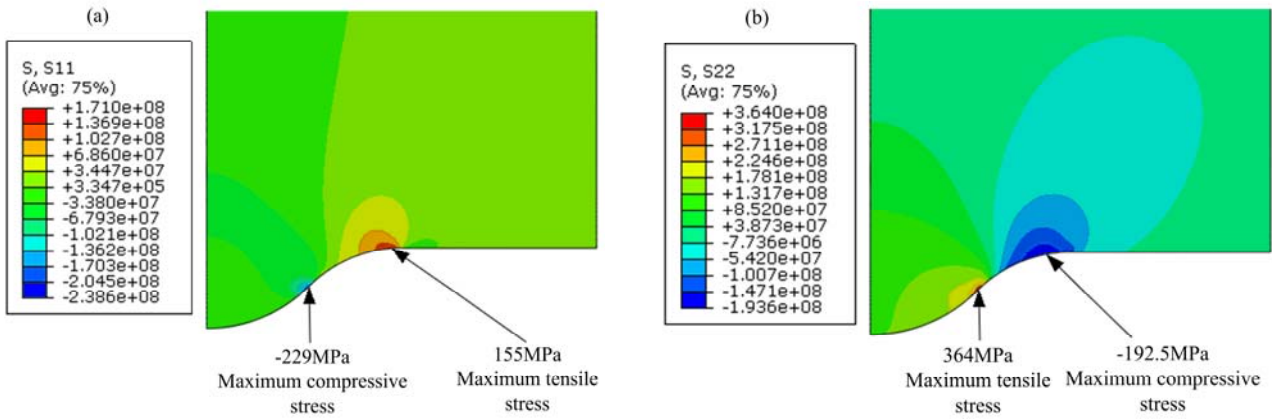


Figure 4. Stress distribution within TC when the TC is intact. (a) in-plane stress ( $\sigma_{11}$ ) and (b) out-of-plane stress ( $\sigma_{22}$ ).

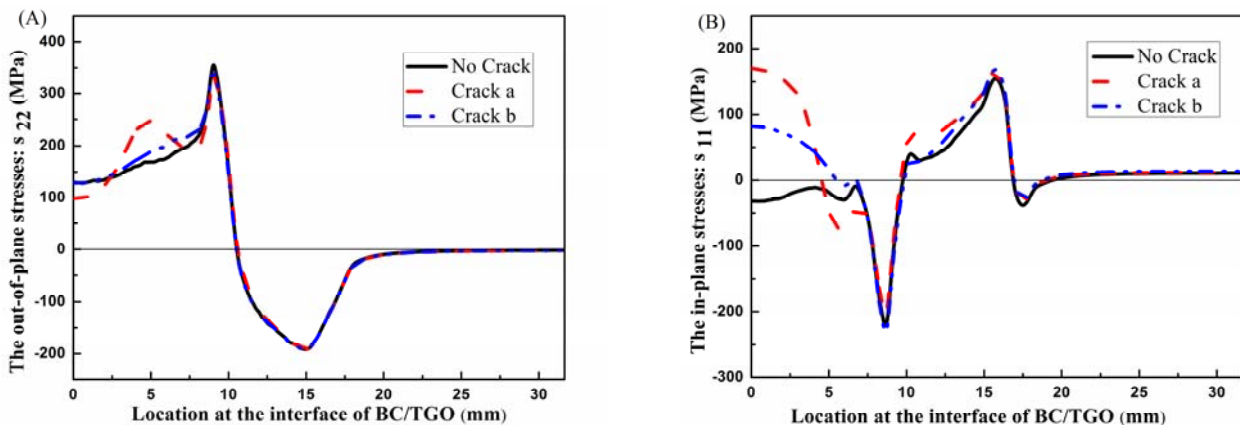


Figure 5. Stress distribution in TC along TC-TGO interface. (A) The out-of-plane stress ( $\sigma_{22}$ ).

(B) The in-plane stress ( $\sigma_{11}$ ).

The distribution of in-plane stress ( $\sigma_{11}$ ) in the intact TC is depicted in Fig. 4a. The compressive in-plane stress can induce the failure of the system by resulting in large-scale buckling [14]. Fig. 4a shows that the compressive  $\sigma_{11}$  mainly occurs in the zones above the instability site and the tensile part distributes around the periphery of the instability zone. Fig. 5B presents the distribution of in-plane stress in TC along the TC-TGO interface under the case a crack existing within TC. The existing of crack within TC makes the stress state in the region above the instability site become tensile from compressive. Especially, when the crack is close to the base of instability site (crack “a”), the tensile stress is significant. Compared to the compressive state of in-plane stress, this tensile state may reduce the probability of buckling occurring. Therefore, the existing of the crack can partly prevent the failure mode caused by buckling.

#### 4.2. The effect of crack length

The influence of the normalized crack length  $L/L_{\max}$  on the instability amplitude defined by  $\delta R_1/\delta R_1^0$  and  $\delta R_2/\delta R_2^0$  is shown in Fig. 6, where  $L_{\max}$  is the maximum crack length used in the calculations, and  $\delta R_1^0$  and  $\delta R_2^0$  are the instability amplitudes when there is no crack within TC. It can be seen that both the magnitudes of the downward displacement  $\delta R_1$  and the upward displacement  $\delta R_2$  increase as the increase of crack length under both cracks case, and the increase rate also increase as the increase of crack length. It indicates that the crack extending would aggravate the instability and make the interface distortion be more significant. Inversely, the large interface distortion also can enhance the capacity of crack extending [3] and finally induce the failure of system. Note that the amplitude change of the displacement instability for the crack “a”, which is more close to the base of instability site, is always greater than that for crack “b”. This result shows that the crack close to the base of instability site has a greater enhancement on the instability. In addition, as the increase of crack length, the amplification of downward displacement  $\delta R_1$  is always greater than that of upward displacement  $\delta R_2$ . From  $L/L_{\max} = 0.5$  to  $L/L_{\max} = 1.0$ , the normalized amplification of  $\delta R_1/\delta R_1^0$  is increased by more than 5 times, which can result in a markedly distortion at the interface. Therefore, the propagation of crack can significantly enhance the interface distortions as thermal cycling, especially that of the crack close to the base of instability site.

#### 4.3. The effect of crack angle

The effect of the crack angle ( $\theta_1$  and  $\theta_2$ ) on the normalized instability amplitude  $\delta R_1/\delta R_1^0$  and  $\delta R_2/\delta R_2^0$  is shown in Fig. 7. Six different crack angles of  $15^\circ$ ,  $30^\circ$ ,  $45^\circ$ ,  $60^\circ$ ,  $75^\circ$  and  $90^\circ$  are used in the calculations for both  $\theta_1$  and  $\theta_2$ . It is demonstrated that the upward displacement  $\delta R_2$  is insensitive to the crack angle. However, the crack angle has a great influence on the downward displacement  $\delta R_1$ . When the angle is relatively small, the  $\delta R_1$  increases as the increase of the crack angle. But when the crack angle makes the crack trend to be parallel the flat interface,  $\delta R_1$  begins to decrease as the increase of the crack angle. From the previous analysis we can see that the propagation of crack within TC is preferential along the direction which is parallel to flat interface [33]. Therefore, when the crack direction is close to the preferential propagation direction, the crack propagation would play a dominant role and the instability of TGO can be restrained. However, even the extending of displacement amplitude begins to slow down when the crack trends to parallel to flat interface, the effect of the crack in this direction on the displacement instability is much greater than that of the crack in the direction which is perpendicular to the flat interface.

Therefore, when the pre-existing crack is introduced within TC, the crack in the direction which is perpendicular to the flat interface is the optimal choice for preventing the large instability.

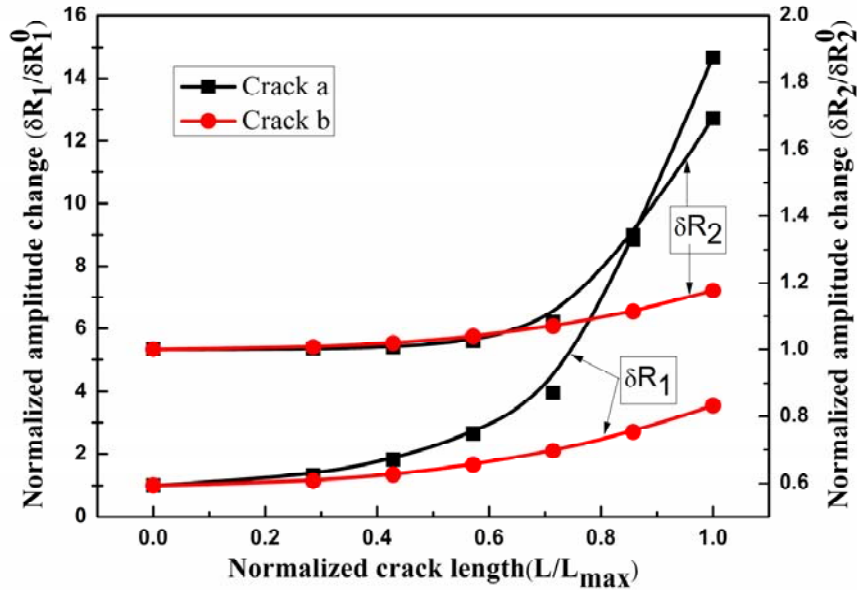


Figure 6. Normalized  $\delta R_1$  and  $\delta R_2$  vs. normalized crack length ( $L/L_{max}$ ).

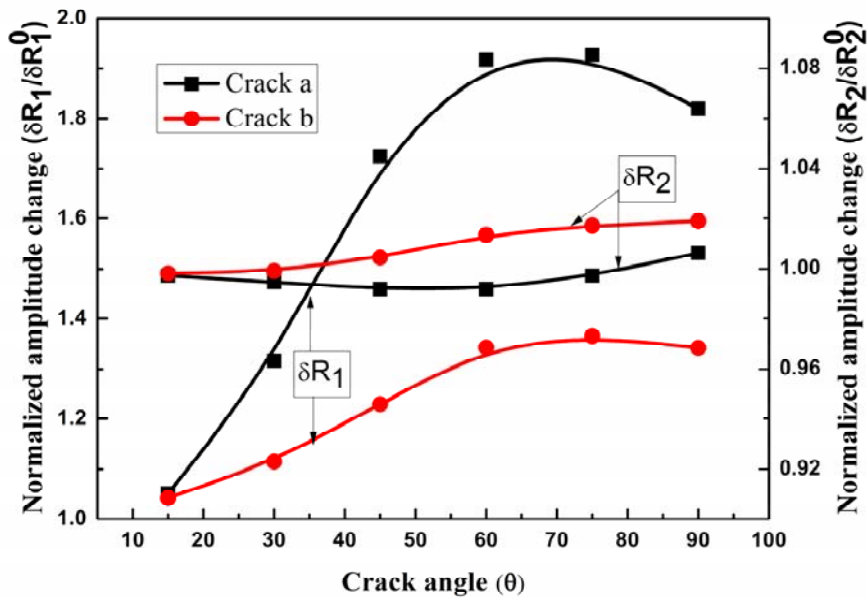


Figure 7. Normalized  $\delta R_1$  and  $\delta R_2$  vs. the crack angle ( $\theta$ ).

## 5. conclusions

The effect of pre-existing microcrack within TC on the displacement instability of TGO in thermal barrier systems is studied by a finite element model with the thermal growth behavior of TGO layer.

The influence of variational crack locations, length and direction on the development of stress and the instability amplitude is discussed. The main results from the calculations suggest:

- (1) The crack within TC would promote the TGO displacement instability significantly, especially the crack close to the instability site.
- (2) The tensile part of the out-of-plane stress, which is responsible for the delamination, mainly concentrates on the zone near the instability site and it can be promoted by the crack existing within TC. However, the compressed part of in-plane stress, which is responsible for the buckling, is restrained by this crack.
- (3) The crack length and direction are two key factors affecting the displacement instability, especially the crack length. As the increase of the crack length, the amplitude of displacement instability increases significantly, which results in a serious interface distortion. The effect of crack direction mainly focuses on the downward displacement instability. The crack in the direction perpendicular to the flat interface is the optimal choice for prevent the large instability.

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