Review

Research Progress of Failure Mechanism of Thermal Barrier Coatings at High Temperature via Finite Element Method

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Abstract: In the past decades, the durability of thermal barrier coatings (TBCs) has been extensively studied. The majority of researches emphasized the problem of oxidation, corrosion, and erosion induced by foreign object damage (FOD). TBCs with low thermal conductivity are usually coated on the hot-section components of the aircraft engine. The main composition of the TBCs is top-coat, which is usually regarded as a wear-resistant and heat-insulating layer, and it will significantly improve the working temperature of the hot-section components of the aircraft engine. The application of TBCs are serviced under a complex and rigid environment. The external parts of the TBCs are subjected to high-temperature and high-pressure loading, and the inner parts of the TBCs have a large thermal stress due to the different physical properties between the adjacent layers of the TBCs. To improve the heat efficiency of the hot-section components of aircraft engines, the working temperature of the TBCs should be improved further, which will result in the failure mechanism becoming more and more complicated for TBCs; thus, the current study is focusing on reviewing the failure mechanism of the TBCs when they are serviced under the actual high temperature conditions. Finite element simulation is an important method to study the failure mechanism of the TBCs, especially under some extremely rigid environments, which the experimental method cannot realize. In this paper, the research progress of the failure mechanism of TBCs at high temperature via finite element modeling is systematically reviewed.

Keywords: thermal barrier coatings (TBCs); finite element method; thermal-mechanical; TGO (thermally growth oxide); failure mechanism

1. Introduction

Since the application of gas turbines in related industrial fields in the 20th century, the research of gas turbines has performed a vital function in promoting the development of national energy. The efficiency of gas turbines has been affected by gas temperature and compressor compression ratio [1]. With the demand for combustion efficiency and thrust weight ratio of gas turbines becoming stricter and stricter, hot-section components have undergone development from alloy to single-crystal nickel-based superalloy materials under the continuous exploration of researchers since the 1940s. The working temperature was also raised from 760 to 1150 °C. Nevertheless, they are still unable to
meet the performance requirements of high temperature resistance, high strength, corrosion resistance, and so on. It needs coating protection to avoid damage of the substrate. With the increase in working temperature, it is more and more difficult to further raise the working temperature of gas turbine material. Thermal barrier coatings (TBCs) and high-pressure air cooling are required to reduce the working temperature of the aircraft (Figure 1). However, the assembly of cooling equipment not only increases the load of the aircraft, but also brings potential safety hazards, which limits the flight distance. Therefore, plasma-sprayed TBCs have become one of the crucial means to reduce the working temperature of the hot-section component of aero-engines and gas turbines. TBC technology has become a core technology to provide cooling to aircraft engines and turbine blades. The existence of TBCs enables working parts to withstand higher temperatures and protects them from wear, oxidation, and erosion. The application of advanced TBCs on the hot-section components of gas turbines can ensure the substrate works at high temperatures, which will significantly improve the thermal efficiency of the aircraft [2,3]. With the development of TBC technology and its wide recognition, it has attracted the attention of quite a few scholars. Carter et al. [4] illustrated the common failure mechanisms found in gas turbine blades, many factors that shorten the lifetime of gas turbine were considered, such as mechanical damage, high temperature damage, high temperature exposure, creep failures, etc. Clarke et al. [5] emphasized that the improvement of thrust-weight ratio and reliability of gas turbines is closely related to the development of thermal barrier coating technology. There is an acute need for high-temperature protective coatings in the fields of aerospace, energy, and the nuclear industry.

Many scholars have carried out various research works on TBCs [2,6–14]. It has been found that the failure caused by TBCs is unavoidable under the conditions of high temperature and long-term usage. During thermal cycling, the failure of atmospheric plasma-sprayed thermal barrier coatings (APS-TBCs) usually occurs in the surface layer near the interface. This is due to the thermal mechanical stress caused by the mismatch of the thermal expansion coefficient between the adjacent layers in the TBCs during thermal cycling. The existing method of APS leads to crack propagation at the interface. With the release of energy in the process of grain growth, transverse or longitudinal cracks are formed. The uneven distribution of cracks will lead to the delamination of coatings during cooling, the coatings on the surface of hot-section component will peel off, thus affecting the service life of gas turbines [15]. Reliability and durability are two key factors determining the service lifetime of TBCs [14]. Reliability requires that the TBCs have strong bonding strength, high thermal insulation, low residual stress, and outstanding high-temperature oxidation resistance. The durability of TBCs requires that the TBCs have a long service lifetime under actual working conditions [13,14]. Distribution of temperature field and residual stress are two important aspects of TBCs under actual application conditions. Effective thermal conductivity or thermal insulation effect is usually calculated by the distribution of temperature field across the whole coatings. The temperature distribution of TBCs can be calculated via finite element method (FEM). Residual stress is also essential to TBCs, and it will affect the failure modes and service lifetime of TBCs. In fact, residual stress will occur in the TBCs during the manufacturing process. Additionally, under the conditions of thermal shock and high-temperature oxidation, residual stress can be also induced, which makes the coating peel off directly. It is a common phenomenon that the coating peeling restricts the wide application of TBCs. TBCs usually operate under alternate cooling and heating conditions. Therefore, improving thermal shock resistance is a direct and effective way to prolong the lifetime of TBCs. With the renewal of the engine, the higher thrust weight ratio leads the TBCs to the direction of ultra-high temperature, low thermal conductivity, and long lifetime. Correspondingly, the research on the structure system and preparation technology of ultra-high temperature TBCs, as well as the characterization of advanced TBCs in a complex working environment need to be further explored [16]. However, the preparation of TBCs with excellent performance via experimental method is a complex process, and there are many unknown factors, which need further exploration. The finite element simulation is helpful to optimize the preparation process and the coating structure, save research time and cost, and make the research work more efficient. Finite element simulation can help us to find the optimal process and the coating structure under specific
target conditions [17]. Before designing excellent TBCs, the layered structure, micro-structure, and related manufacturing technology of various TBCs should be understood. The moving process of the spray gun in plasma-sprayed TBCs is denoted in Figure 2. The following is the research status of the dominating factors affecting the failure modes and life evaluation of TBCs.

![Figure 1. Hot-section component model of thermal barrier coatings.](image1)

Figure 1. Hot-section component model of thermal barrier coatings. (a) The interior appointments of the turbine; (b) Yttria stabilized zirconia (YSZ) thermal barrier coatings; (c) thermal barrier coatings (TBC) coated on the turbine blade. Adapted with permission from [13]; Copyright 2016 Elsevier.

![Figure 2.](image2)

Figure 2. (a) The microstructure of the as-sprayed coating (b) Raster pattern in the x–y plane for one cycle of gun movement [18].

2. Structure and Preparation Technology of TBCs

2.1. Structure Model of TBCs

TBCs have been widely used in many industrial fields related to energy and power because of their excellent high-temperature resistance, high thermal insulation, and corrosion resistance. TBCs are an important inorganic coating, which consists of the ceramic oxide layer and bond-coat. While spraying on the base of superalloy material, the influence of high temperature on the hot-section components has been reduced, thus the service temperature is reduced and the working efficiency of gas turbine has been improved [19]. The common TBCs can be divided into three types: double-layer structure coatings, multi-layer structure coatings, and functional gradient coatings, as shown in Figure 3.
2.1.1. Double-Layer Structure Coating

As for the classical double-layer structure coating, TBCs are composed of a ceramic layer and bond-coat. The thickness of the ceramic layer is generally less than 300 µm, and the thickness of the bond-coat is generally less than 150 µm. The ceramic surface made of oxide ceramics has the functions of heat insulation and corrosion resistance. In addition, the bond-coat consisting of metal alloys can enhance the bonding strength between the substrate and the ceramic surface and weaken the mismatch of thermal expansion between the two layers, and at the same time enhance the high-temperature oxidation resistance of the substrate [20].

2.1.2. Multi-Layer Structure Coating Model

Multi-layer structure coatings are composed of a ceramic layer, bond-coat, and multi-layer immediate layer with different functions, in which the immediate layer can include a self-healing layer and/or an insulation layer.

Double-layer TBCs are a widely used coating structure model because of their high thermal insulation, high interfacial bonding strength, and relatively low preparation cost. However, the thermal and physical properties of the ceramic layer and the bond-coat are quite different. During cooling from the high temperature, residual stress is easy to induce in the coating, and cracks occur easily at the interface, which eventually contributes to the ceramic layer falling off and the service lifetime would not reach the expected value. Moreover, the service process of TBCs at high temperature and the complex environment of high-pressure results in many unfavorable factors which can accelerate the failure of the TBCs, such as thermal stress, mechanical stress, chemical reaction of coatings at high temperature, and thermal corrosion. In order to prolong the service lifetime of coatings and reduce the failure of the coating under various factors, the concept of multi-layer TBCs has been proposed. Compared with double-layer TBCs, multi-layer TBCs add several layers with different functions between the ceramic layer and the bond-coat. The interlayer coating can be a sealing layer, a heat insulation layer, a thermal stress control layer, or a non-diffusion layer, etc [21]. Different multi-layer structure coatings have different bond-coats, and their properties are also different [22]. For example, the blocking layer that has been fabricated by Al₂O₃ can reduce the diffusion of oxygen atoms, prevent oxidation reaction in the coating, and slow down the oxidation failure of the bond-coat.
2.1.3. Functional Graded Thermal Barrier Coatings Model

The structural characteristics of functional graded coatings are as follows: the composition of bond-coat and ceramic material between the coatings from metallic substrate to ceramic surfaces exhibit continuous gradient changes [23].

In view of the premature failure of ceramic coatings, functional gradient coatings were proposed by Japanese scholars in the 1990s. The structure and mechanical properties of functionally graded coatings are continuous, with the composition of the coatings due to the gradient change between the ceramic layer and the metallic substrate. This continuous structure can effectively alleviate the thermal stress between the ceramic layer and the metallic substrate, and effectively improve the thermal shock resistance of the coating [24]. Functionally graded TBCs have excellent thermal shock resistance compared with double-layer TBCs, but the preparation is difficult and the repeatability limits the practical application of functionally graded TBCs.

Besides the above three coatings, there are also coatings structure models such as thick coatings and double ceramic TBCs. Thick coatings have a large thickness and good thermal insulation, which can be used to improve the combustion temperature of fuel, such as double ceramic TBCs. In addition, they play an important role in improving fuel combustion temperature and reducing exhaust emissions. Nevertheless, the increase in thickness also leads to the increase in temperature gradient and thermal stress in the coating. The increase in thermal stress and the temperature gradient will cause failure of the coating far away from the substrate interface before the interface cracking. This design of a double ceramic layer structure combines the advantages of two different ceramic materials and complements each other’s shortcomings. The structure of double ceramic coatings is to add an intermediate layer with a small difference in thermal expansion coefficient between the zircon coating and the transition layer. Wang et al. [14] discovered that the thermal shock resistance of La2Zr2O7/YSZ double ceramic coatings has significantly improved compared to that of single La2Zr2O7 coatings. La2Zr2O7/8YSZ double ceramic coatings were fabricated by Xu via Electron Beam-Physical Vapor Deposition (EB-PVD) [25]. Besides, the thermal cycle test at 1373 K in an air furnace indicates that the double ceramic layer TBCs have a higher thermal cycle lifetime than that of single ceramic layer TBCs (LZ and YSZ). The research shows that this design can greatly prolong the thermal cycle lifetime of coatings and significantly increase the service temperature of coatings. It will be one of the effective ways to flourish ultra-high temperature TBCs in the future [26].

2.2. Preparation Technology of Thermal Barrier Coatings

The preparation methods of TBCs include electron beam-physical vapor deposition, (EB-PVD) [27], plasma spray physical vapor deposition (PS-PVD) [28], and atmospheric plasma spray (APS) [29], as shown in Table 1.
Table 1. Comparison of EV-PVD, PS-PVD, APS.

<table>
<thead>
<tr>
<th>YSZ</th>
<th>Microstructure</th>
<th>Failure Mechanism</th>
<th>Finite Element Model</th>
<th>Experiment Model</th>
<th>Reference</th>
</tr>
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<tbody>
<tr>
<td>EB-PVB</td>
<td>Typical characteristic with columnar grain, the adjacent columnar grains are leaned with each other.</td>
<td>◆ In the process of thermal shock cooling, cracks are easy to form from pores and propagate along the interface, leading to premature failure of TBCs.</td>
<td><img src="image1.png" alt="Image" /></td>
<td><img src="image2.png" alt="Image" /></td>
<td>[3,8,27–33]</td>
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<tr>
<td>PS-PVD</td>
<td>Typical characteristic with feather-like columnar</td>
<td>★ The gap and pore are the main defects which exist in the columns. With the immersion of high-speed corrosives, the coating will be corroded quickly, resulting in the failure of the coating.</td>
<td><img src="image3.png" alt="Image" /></td>
<td><img src="image4.png" alt="Image" /></td>
<td>[3–8,28,30–33]</td>
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<tr>
<td>APS</td>
<td>Exhibit lamellar structure characteristic. Micro-pores and micro-cracks are distributed at random in the ceramic</td>
<td>▲ A continuous crack network can form according to the connectivity of inter-splat crack and intra-splat crack, which will result in the crack growth along the lamella interface or through lamella interface.</td>
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<td><img src="image6.png" alt="Image" /></td>
<td>[8,13,16,34–38]</td>
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2.2.1. EB-PVD

EB-PVD is a commonly used technology for preparing TBCs. Its working principle can be depicted as follows: after the vacuum chamber is vacuumed to a certain degree, the electron gun will shoot an electron beam, bombard the evaporated materials in the water-cooled crucible, and the evaporated materials will condense to the preheated substrate surface in the form of atoms or molecules, forming a columnar structure of coating on the substrate. The pores between the columns and the interstices in the column provide favorable conditions for the transfer of heat and oxygen, resulting in a decrease in heat insulation performance and the easy oxidation of the coating structure, which is conducive to alleviating the thermal stress caused by the difference in thermal expansion coefficient of the coating, and improve the anti-thermal fatigue and thermal shock resistance of the materials [16,38,39]. However, it cannot be ignored that due to the existence of a large number of pores perpendicular to the coating surface and the intragranular gap between the adjacent columnar grains, it will not be conducive to the thermal insulation of the coating. In the process of thermal shock, cracks can easily form pores and propagate along the interface, leading to premature failure of TBCs. Evans et al. [40] investigated the composition of the coatings and their thermal properties using EB-PVB. Van sluytman et al. [39] prepared ZrO$_2$–Y$_2$O$_3$–Ta$_2$O$_5$ TBCs. It was found that the coating sintered and contracted under the constant oxidation temperature of 1450 °C, resulting in the generation of residual stress in the TBCs, leading to premature peeling failure of the coating. Therefore, as for the TBCs prepared via EB-PVB, the separation of different layers can lead to the final failure.

2.2.2. PS-PVD

Plasma spraying-physical vapor deposition (PS-PVD) is a new multi-functional film and coating preparation technology based on low-pressure plasma spraying. This technology combines the technical advantages of APS and EB-PVD and can be used for vapor deposition in the form of spraying. PS-PVD uses a high-power plasma spray gun (180 kW) to work under ultra-low pressure (150 Pa). Under this condition, the plasma jet of PS-PVD expands rapidly, making its length up to 2000 mm and diameter up to 400 mm. It can realize gas-liquid-solid multiphase coating deposition and obtain non-line-of-sight deposition [28]. Rare earth doped zirconia (ZrO$_2$: 1.7Y$_2$O$_3$–1Gd$_2$O$_3$–1Yb$_2$O$_3$ at.%)) TBCs were fabricated by Deng [28] via PS-PVD. There was a large quantity of pseudo-columnar crystal structures in the coatings. The pseudo-columnar crystal size in PS-PVD is obviously large and resistant to fracture. However, the gaps and pores are the main defects which exist in the columns. With the immersion of high-speed corrosives, the coating will be corroded quickly, resulting in the failure of the coating.

2.2.3. APS

Atmospheric plasma spraying (APS) [22,41] can produce the plasma arc which is driven by direct current as a heat source. Actually, high-energy is the typical characteristic. Additionally, powder is suspended in a carrier gas (inert protective gas). The coating is formed by impinging powder particles on the surface of the substrate during spraying. The microstructure of the coating is related to the properties of the spraying material, spraying parameters, and surface temperature of the substrate. In order to prevent a turbine blade from being corroded, plasma spraying technology was applied to prepare 8YSZ coating by Mack [42]. The formation and growth of cracks under thermal cycling were elucidated by combining scanning electron microscopy (SEM) with the X-ray diffraction (XRD) technique, and the corrosion velocity was observed by calcium-magnesium-aluminum-silicate (CMAS) deposition. It was found that in a short period of time, there was an obvious CMAS attack on grain boundaries, but the interaction between YSZ and invaded CMAS was without direct influence on the pore structure and inner surface density. The densification of YSZ microstructures was observed only at the later stage if a marvelous amount of CMAS was immersed. Wang et al. [13,14] prepared 8YSZ TBCs by APS. The effects of horizontal and vertical cracks on the stress around the TGO (Thermally
Growth Oxide) layer during thermal cycling were studied. Dong et al. [43] fabricated YSZ coatings by APS, finding that TGO with different thickness was prepared by controlling the isothermal oxidation time of the bond-coat. Thermal cycling tests were carried out for different thicknesses of TGO at 1150 °C, the duration of each cycle was 240 s. The results indicated that the YSZ coating has strong adhesive strength, and excellent thermal shock resistance.

However, the influence of failure is related to TBC structure, the typical microstructure feature of APS-TBCs depends on its typical lamellar structure, the low bonding strength is due to lots of void defects in the APS-TBCs. Generally, the pores, the inter-splat cracks, and intra-splat cracks existing in YSZ coating would affect the quality of APS-TBCs. Besides, the pores and inter-splat cracks distribution affect the interface bonding rates, which are attributed to the process of APS. In APS-TBCs, a continuous crack network can be formed according to the connectivity of interlaminar and intralaminar cracks, which will result in crack initiation and propagation along the lamellar or through-lamellar direction.

A host of research results have showed that the cracks exist in the top-coat layer or near the TC (top-coat)/TGO interfaces in APS-TBCs. During the thermal shock, these cracks can propagate along the stratiform interface or through lamella under complex stress states [44–46]. The spallation of coating frequently take place owing to the crack initiation along the layer interface, which is accountable for the failure of APS-TBCs. As the spread of these cracks is random and irregular, it is very urgent to determine the crack propagation behavior and coalescence mechanism [36].

3. The Factors Affecting the Service Lifetime of TBCs

3.1. TGO

Hundreds of different types of coatings are used to protect various engineering materials from corrosion, wear, and erosion, and to provide lubrication and insulation. TBCs are regarded as the coating with the most complex structure among coatings. They must work in the high-temperature environment of aircraft and industrial gas turbines. Due to the diffusion and reaction of oxygen and aluminum, an additional layer called TGO (thermally-grown oxide) is formed at the interface between TC and BC (Figure 4). For the whole high-temperature oxidation, the oxides were primarily Al₂O₃ and a small amount of Cr and Co oxides at the TC/BC (bond-coat) interface [47]. During the development of TGO, the local accumulation of TGO has a profound effect on the stress distribution near the interface. Understanding the formation and stress distribution of TGO is the basis for predicting TBC’s lifetime, which plays an important role in preventing further oxidation and corrosion of TBCs [11,48]. Due to the diversity of reaction mechanisms in the oxidation process of TGO, many studies have illustrated that TGO grows rapidly at the initial stage of oxidation. This is attributed to the following reason: with an increase in temperature, Al₂O₃ can be produced freely, resulting in the uneven growth of the thickness of TGO and an increase in the roughness of TGO, and the accumulation of residual stress with the increase in thickness, which results in growth stress in the thin layer of TGO [3]. The results reveal that coating failure usually occurs at the TGO/BC interface. This phenomenon is mainly due to the large stress produced by the growth of TGO layer and its interface [49].
Oxidation is accompanied by growth strains and associated stresses; the strain represents the overall volume increase upon converting the alloy to Al₂O₃—when the growth strain is large enough, the stress suppresses the internal TGO formation, forming a critical stress. Once this value is exceeded, it may cause interfacial crack generation and propagation along the TC/TGO/BC interface, and the service lifetime is affected. As shown in Figure 5, Evans [3] analyzed the intrinsic failure of TBCs, and the growth of TGO layer is the key issue of coating durability. However, the thickness and morphology of TGO vary with the increase in service time at high temperature. Therefore, it is necessary to study the evolution of TGO layer during thermal exposure. Influenced by the diversity of the high-temperature oxidation mechanism, the oxidation diversity of TBCs is extremely complex, including the composition of materials, the preparation process, and the thickness of coatings. Therefore, different thicknesses and shapes of the TGO layer are formed, which is of great significance to stress distribution around the TGO layer and to the life prediction of TBCs. During the thermal shock cycle, growth of TGO is observed, and the multilayer accumulation of TGO is observed in the protrusion of the surface roughness of the TBCs. The accumulation of TGO results in the cracking of the top layer [30]. This phenomenon is more obvious for TBCs fabricated by APS [43,51,52] (Figure 5). According to previous primary simulation work [53], we can also observe a similar phenomenon that the growth rate of TGO near the peak region is higher than that near the valley region. Che et al. [54] investigated that TGO grew unevenly at the peaks and valleys of the rough top coat/TGO interface after isothermal exposure at 1050 °C. TGO grew exponentially near the peaks and valleys, and TGO was thick at the peaks, where there are large tensile stresses, uniformity, and unevenness at the peaks. There is a significant difference in the distribution of stress between uneven and uniform TGO. For uneven TGO, the maximum out-of-plane stress of peak and valley increase 200%, and the maximum tensile stress along the interface of the TGO/surface layer is smaller than that of uniform TGO. Moreover, compared with TBCs which were serviced under a uniform temperature field, in the case where TBC is subjected to a thermal gradient, the gradient will affect the growth rate and stress distribution of TGO. Thus, it is of significant importance to consider the failure modes of TBCs under uniform and non-uniform temperature fields. Ranjar-Far et al. [55] considered a nonhomogeneous temperature distribution. The results indicated the residual stress distribution was significantly affected by thermal gradient. Based on the TCF experiments, Schulz et al. [56] observed that the spallation of the TBCs is mainly correlated with TGO formation that is influenced by uniform temperature field, and the failure of the EB-PVD TBCs was caused by TC/TGO interfacial crack propagation, which easily results in the spallation and buckling of the TC layer. To investigate the effect of the thermal gradient on the TBC failure modes, the growth of the TGO layers was taken into account by Shi [4]. The results indicated that the thermal gradient affected the vertical stress initiation and propagation. Meanwhile, the interfacial cracking behavior...
was dominated by TGO growth stress. The thermal protective performance and oxidation resistance of the TBCs were influenced.

Dong et al. [43] discussed the influence of TGO with different thicknesses on the failure behavior of the TBCs. The results of thermal cycling tests of APS-TBCs with different initial thicknesses of TGO indicated that with the increase in the thickness of TGO, the thermal cycling life decreases with the increase in the power function, and there is a critical thermal cycling life which decreases significantly with the increase in TGO thickness. As shown in Figure 6, moreover, the typical failure modes were affected by TGO thickness, making the crack generation and propagation along the TC/TGO/BC interface. Therefore, the thickness of TGO has a significant effect on the thermal cycle life of TBCs, and the uneven distribution and accumulation of TGO will also affect the service lifetime of the coatings. To further investigate the effect of the service lifetime of TBCs, the thermal expansion mismatch should be considered.

**Figure 5.** Schematics indicating the TGO growth modes and its implications for the development of growth stresses. Reprinted with permission from [8]; Copyright 2001 Elsevier.

**Figure 6.** Stress components and equivalent plastic strain (PEEQ) at the ambient temperature considering the interface crack: (a) Mises stress, (b) S11, stress in x direction, (c) S22, stress in y direction, and (d) PEEQ, equivalent plastic strain. Reprinted with permission from [57]; Copyright 2017 ASME.
3.2. Thermal Expansion Mismatch

The thermal mismatch stresses near the TGO layer occur during thermal cycling, which is due to the great differences in physical, thermal, and mechanical properties of adjacent layers. The damage and failure of TBCs are related to the mismatch of the thermal expansion coefficient. The cracks generated by the residual stress may nucleate and expand to the interface, which will affect the stress state in the TBCs [54,58]. Jiang et al. [57] have pointed out a large local tensile stress in the TGO coating during cooling, and a crack occurs at the peak value of the TGO interface. In addition, Fan et al. [59] have discussed the effect of TGO on the multiple surface cracking behavior in APS-TBCs. The driving force of the periodic surface crack and the mismatch of the crack propagation path were discussed by using the extended finite element method (XFEM) and the periodic boundary conditions. The stress distribution was calculated and the crack propagation path was simulated by XFEM (Figure 7). The results indicate that the elastic modulus of the TGO layer plays a significant role in controlling the strain energy release rate. The related fracture mechanism was mainly controlled by the mismatch between the top coating and the bond-coat, which can be used as a guide for the well-designed strain-resistant APS-TBCs.

Huang et al. [60] considered the effect of interface roughness on strain energy release rate (Strain Energy Release Rate) and surface cracking behavior in APS-TBCs by XFEM. The driving forces of multiple surface cracks in the coating/substrate system were predicted and presented. It was found that the interfacial roughness has a significant effect on the surface roughness, interfacial stress distribution, and propagation modes of cracks. Sfar et al. [61] established a TBCs failure model, the residual stress of the TC region at the peak of TC/TGO interface due to thermal mismatch failure was studied, which was used to evaluate the interface toughness or to measure the initiation of cracks. The stress concentration near the TGO layer was discussed when the vertical crack was above the peak value of the TGO layer by establishing the TBCs failure model. Compared with the horizontal crack, the vertical crack could be partially released, resulting in stress concentration near the TGO layer. When horizontal cracks exist, the maximum tensile stress is located at the peak of the TGO/BC interface. When there is a vertical crack, the stress concentration tends to appear near the crack tip. The effect of horizontal cracks and vertical cracks on the stress around TGO is obviously different. The existence of vertical cracks can significantly reduce the maximum tensile stress concentration in the TGO layer. Tolpygo et al. [5] observed that the thermal mismatch of 7YSZ coating occurred during the cycling furnace test, and horizontal and interfacial cracks inclined near the TGO layer, resulting in coating failure. In order to study the failure mechanism caused by TGO, Wang et al. [12,13,16,62,63] have done a generous of research on crack...
propagation in previous reports. Including the study of horizontal cracks, vertical cracks, internal cracks, or interfacial cracks in coatings, the results indicated that the stress concentration is related to the location of vertical and horizontal cracks, as shown in Figure 8, and the crack length also affects the failure of TBCs [5,13,14], especially for the thick thermal barrier coatings (TTBCs) fabricated by APS, vertical cracks (also known as segmentation cracks) are distributed in the top-coat (ceramic layer); usually, the length of segmentation cracks is more than half of the thickness of the coating. For the thickness of the top coating, the existence of segmentation cracks will reduce the stress concentration of TTBCs, thereby increasing the strain tolerance of the coating [58,64,65]. Therefore, it is useful to ensure a significant improvement in thermal shock resistance. Although segmentation cracks are not conducive to reduce thermal conductivity, the thickness of TBCs is enough, which will ensure that TBCs still have a high thermal insulation effect [5]. In fact, the stress level and distribution play a crucial role in controlling the failure of TBCs during thermal shock. The special microstructure of TBCs affects the stress distribution and maximum stress level of TBCs. In particular, there were many segmentation cracks in the TC layer, which released more or less energy and caused the stress concentration. Besides, the geometric characteristics of segmentation cracks will affect the failure behavior of materials. Although the existence of cracks can increase the strain tolerance and improve the thermal shock resistance of materials, the propagation of segmentation cracks is still the main cause of coating failure. Dong et al. [66] studied the distribution of temperature on a YSZ-free surface during crack coalescing via FEM, then the influence of sintering of YSZ induced by heat-transfer overlapping on energy release rate was quantificationally evaluated. Fan et al. [67] investigated the effect of the periodic surface cracks on interfacial fracture of TBC systems via cohesive zone model (CZM). The results indicated that the spacing of surface cracks has a significant effect on the initiation and propagation of cracks in TBC systems. For short interfacial cracks, it can be concluded from the simulation results that suitable high surface crack density can improve the durability of the TBC system. The delamination behavior of the interface often occurs when the vertical crack propagates to the interface. Therefore, controlling the delamination behavior is very important for delaying the failure of TBCs. Bake et al. [68] discovered the initiation and propagation of cracks near the interface, and the direction of crack propagation tended to the BC/TGO interface. The results indicate that the morphology and deformation of TGO play an important role in the nucleation and propagation of cracks. Wei et al. [69] analyzed that an increase in the transverse growth strain of TGO would lead to premature peeling of coatings, and the bond-coat and creep of TGO have only a slight shrinkage effect. If the stress of TGO is low, the cracking of ceramics occurs. However, growth of the TGO tends to increase the interfacial stress within the TBC system and would affect the surface crack density. Zhu et al. [70] found that cracks easily propagate from the surface to the interface with the surface crack density decreasing, while the cracks generate and propagate along the surface with high surface crack density. The saturated crack density decreases with the increase in ceramic coating thickness. Furthermore, the surface crack density has a significant effect on the initiation and propagation of interface cracks. The interfacial delamination length decreases with an increase in surface crack density, and the interfacial delamination would not occur before reaching the critical surface crack density. It can delay the delamination of the coating and improve the thermal shock resistance and durability of the coating with reducing the thermal matching and increasing the interfacial adhesion strength of the coating. The TGO growth rate, which may accelerate the failure of TBCs, was affected via oxidation temperature and time. Experimental simulation was confirmed by Trunova [71]. The failure modes and lifetime of the APS-TBC were influenced, the large extent on the thermal load conditions were taken into account. It promotes delamination cracking in the TBC close to the TBC/TGO interface during thermal cycling. The failure crack path to transfer to TGO was affected during the introduction of high temperature residence time, and caused the final failure to be almost completely within TGO. The experimental results indicated that the observed damage evolution was mainly caused by the formation of cracks, the connection of single cracks, and crack propagation. Within a certain residence time, the degradation of the TBC system is affected by the degradation process connected with the adhesion layer, and damage accumulation is influenced
by TGO growth stress, leading to a reduction in cycle lifetime. In addition, the toughness value is affected by cracks during the thermal cycle; it is possible to learn from the available research findings that several crack propagation paths, such as crack bridging, will enhance fracture toughness [72]. Considering the influence of high temperature and TBC exposure time, a model of interface fracture toughness of thermal barrier coating is proposed. The model is expressed in the form of an Arrhenius type showing temperature-dependent characteristics, and also shows the dependence of the density of microcracks distributed along the interface of the coating. As the experimentally measured microcrack density exhibits thermal cycle-dependent behavior, therefore, the proposed interface crack toughness model was used to explain the experimentally obtained toughness value. Kiyohiro et al. [73] observed that the area and thickness of TGO in blasted TBC (B-TBC) specimens is much lower than that of the non-blasted TBC (S-TBC). An indentation test was performed to evaluate the TC/BC interface fracture toughness ($K_{IFC}$), confirming that the $K_{IFC}$ of the B-TBC specimen was significantly higher than that of the S-TBC specimen. These results indicate that grinding and sandblasting effectively improve the oxidation resistance and adhesion strength of the TBC system. Therefore, the microcracks caused by thermal mismatch failure are an important factor for evaluating interfacial toughness or predicting crack initiation.

![Figure 8. Crack propagation paths in the TBCs for different crack positions and TGO with different elastic modulus: (a) peak, $E_{TGO} = 400$ GPa, (b) middle, $E_{TGO} = 400$ GPa, (c) valley, $E_{TGO} = 400$ GPa, (d) peak, $E_{TGO} = 40$ GPa, (e) middle, $E_{TGO} = 40$ GPa, and (f) valley, $E_{TGO} = 40$ GPa. Reprinted with permission from [59]; Copyright 2012 Elsevier.](image)

### 3.3. Roughness of the Interface

The effect of interface roughness on the evolution of TGO thickness and growth stress was also investigated, which showed the effects of growth stress evolution in the thermally grown oxide on the failure mechanism of TBCs. During thermal load, the failure of plasma-sprayed TBCs frequently occurs in the top coatings near the interface. Therefore, it is necessary to study the non-uniform growth mechanism of TGO on the rough interface. Inhomogeneity of the temperature field results in inhomogeneity and roughness of TGO. With the increase of the roughness, the thickness of TGO increases unevenly during the growth of TGO. The rough interface not only causes inhomogeneous growth of TGO, but also affects the stress distribution of TBCs (Figure 9). A lot of research has been done by Evans [3,7,8], and it was found that the durability and stability are limited by delamination along the interface between the TGO and the bond-coat. The interfacial cracks at BC/TGO/YSZ tend to produce energy release. As rumpling is suppressed, the mode delamination is related to the rate of energy release. Actually, as the energy release rate is equal to the type II toughness of the interface, it was found that the lower limit of TGO leading to delamination can be predicted. However, this method of predicting the critical thickness has not been realized due to type II toughness being well-known and difficult to measure. Meanwhile, Shen et al. [74] observed that the thickness of TGO in the valley area
The interfacial roughness also has an obvious effect on the residual stress of TGO and the lifetime of TBCs, the large residual compression in the thermally grown oxide near the interface [8]. In addition, the thermal activation creep process is deformed under high-temperature oxidation. Wang et al. [16,78] characterized the failure behavior of APS-TBCs under the three-point bending (3PB) test using acoustic emission (AE) technology. The results indicated the changes in acoustic emission parameters (number of acoustic emission events, amplitude of acoustic emission, and energy of acoustic emission) as well as stress versus strain during thermal load. The change of curve has a good correspondence. The results of AE analysis and cross-section observation indicated that main cracks tend to propagate towards the TC/BC interface. The actual failure of APS-TBCs is due to the shedding of the metallic coating on the substrate, and the propagation of horizontal cracks along the interface of the substrate/bond-coat under bending moment. Sun et al. [79] compared different samples using real three-dimensional morphologies via finite element modeling, and pointed out that this modeling method is an effective tool to obtain valuable research progress of stress distribution in TBCs. The results of finite element analysis indicated that the residual stress of TBCs is driven by the shear stress and the axial stress of La2Zr2O7 (LZO). The failure of TBCs originates from the corner and propagates parallel to the inherent layered structure of APS-TBCs. The actual failure mode and cross-sectional SEM morphology verified the failure mechanism. Importantly, the local stress changes significantly due to the inhomogeneous growth of TGO. Finite deformation would not be neglected in the oxidation process. Therefore, a theoretical model of oxidation stress based on finite deformation was established, and the effect of a rough interface on stress state was studied. Besides, the local accumulation of TGO will have a profound impact on the stress distribution near the interface, and the stress field of the rough interface will also change the growth rate of TGO at different locations (Figure 10). In a word, the rough interface leads to uneven growth of TGO, and uneven growth leads to increased roughness of TGO. The roughness of TBCs has a significant impact on stress distribution, the failure mechanism, and service lifetime.
3.4. Foreign Object Damage

TBCs used on many hot-section components of aero-turbines are faced with various adverse conditions in the process of service. One of the special conditions that should be paid attention is foreign object damage (FOD). In this case, the hard foreign matter particles often found in the air path of the operating aero-turbine, which are impacted by the leading edge of the High Pressure Turb (HPT) blade, even if such a single impact will occur, lead to crack propagation of the local TBCs, thus eliminating thermal protection on the surface of the hottest part of the whole engine. FOD particles inhaled or released in the gas turbine may collide with coated components and cause the failure of TBCs (Figure 11). Rotating blades are most vulnerable to impact damage because their high rotational speed result in large particle/TBC impact velocity, although the velocity associated with the particle itself is relatively low [40]. Lots of studies have shown that the conditions leading to FOD in jet engines are complex, and the impact angle, impact velocity, particle size, particle composition, and material temperature are jointly affected. TBCs were affected by the foreign body damage (FOD) particles via finite element method, considering a diameter of 4 mm, the incident angle of foreign body and blade temperature affecting the damage analysis during impact process was studied. It was found that the impact perpendicular to the surface is the most dangerous [80]. Rahaman et al. [81] observed that a modulated TBC structure can better withstand impact damage. As shown in Figure 10, the results showed that cracks mainly occurred along the lamellar interface, the visible delamination of TBC observed near the edge of coating. Larsen [82] provided that the depths of FOD damage date follow the Weibull probability distribution. Although a few measurement depths exceeded 1 mm, most damages were in the range of 0 to 400 μm. According to previous studies [82], it was found that these FOD events would not directly lead to failure, the type of damage that they represent should be considered in any design criteria developed to deal with FOD. Moreover, the information provided represents the most widely known data about the size of actual foreign body damage to fans and compressor blades. More research is needed to understand how FOD may affect component failure under high

Figure 10. (a–c) shows the distribution of the normal stress $\sigma_{22}$ at room temperature after 100 cycles in the defect-free model, porous model, and lamellar model, respectively. Similarly, (d–f) shows the shear stress $\sigma_{12}$ distribution in the corresponding models. Reprinted with permission from [36]; Copyright 2019 Elsevier.
cycle fatigue conditions. An experimental simulation was conducted by Peters et al. [83], studying the role of such foreign body damage affecting the fatigue crack growth threshold and large and small crack early crack growth in fan blade alloys. The FOD was simulated by the high-velocity (the sizes of these hard particles are in the millimeter regime, with impact velocities determined primarily by the blade speed and in the range of 100–350 m/s) impact of steel spheres on a flat surface, which was found to markedly reduce the fatigue strength, primarily due to earlier crack initiation. To further investigate the effect of the service lifetime of TBCs, the CMAS corrosion of TBCs should be considered.

Figure 11. Image of the leading edge of an engine-run high-pressure turbine blade showing severe foreign object damage. Note the large gray region which indicates bond coat exposed by complete removal of the TBC. Reprinted with permission from [40]; Copyright 2012 Elsevier.

3.5. CMAS Corrosion of Thermal Barrier Coating

The faults of aircraft in flight are mostly due to the high temperature of turbine inlet. The siliceous minerals (dust, sand, and volcanic ash) in the air are mostly composed of CaO, MgO, Al₂O₃, SiO₂, and other mixed oxides (CMAS). They are sucked into an aircraft engine before CMAS and engine components occur at 1240–1260 °C. In the reaction, the molten CMAS will adhere to the TC surface and penetrate into the columnar gap of the molten phase. Then, CMAS solidifies into hard zone during cooling, which changes the mechanical properties of top coat. Erosion of the coating by both ingested particles, from the operating environment and particles as it degrades, is a perennial source of concern, a great deal of research has been done already [4,6]. Cai et al. [84] discovered that the permeation of CMAS into TC changes the stress distribution around the tissue and induces the formation of cracks. Moreover, the permeation of CMAS would lead to material discontinuity, resulting in a slightly higher stress level around the microstructure of the melted CMAS/TC interface, CMAS permeable layer, and TC/BC interface (Figure 12).

Secondly, creep of aero-engine components will occur during long-term operation at high temperature, and the deformation may contact or squeeze other components, resulting in reduced efficiency of the turbine. Therefore, the serious consequences of failure caused by CMAS are receiving more and more attention. Wu et al. [85] found that the TC coating at the interface between CMAS and YSZ was partially dissolved in CMAS, which induced the phase transformation of YSZ coating from tetragonal phase to monoclinic phase, and further resulted in the porosity and thermal conductivity of the coating decreasing. Su et al. [86] simulated the effect of CMAS penetration on the delamination crack of EB-PVD-TBCs at interface by the finite element method. The immersion of CMAS into the EB-PVD-TBCs columnar gap increased the in-plane modulus of the top coat. With the increase of the in-plane modulus of top coat, the tensile stress level of delamination cracks above the interface decreased. When the shear stress level decreases, the delamination crack tends to increase when the delamination crack extends to the bending interface. However, once the crack extends to a flat
edge, CMAS penetration will begin to enhance its growth and the spallation of the coating will occur (Figure 13). Zhang et al. [87] pointed out that CMAS penetrates into TBCs, and produces transient thermal stresses due to different thermal expansion coefficients. It is easy to cause high in-plane tension when CMAS penetrates into TBCs. The stress produced by the rapid cooling of the top coat promotes the propagation of vertical cracks from the top surface to the bottom of the top coat. At the same time, the accumulation of tensile stress in the outer plane makes the horizontal cracks easily appear at the interface between the penetrating and non-penetrating areas of CMAS. Yang et al. [88] found that the thicker the CMAS deposited, the easier cracks formed at the YSZ/BC interface during cooling. Kim et al. [89] discovered that vertical cracks and holes appeared in TBCs during thermal shock cycles, which had a significant impact on thermal fatigue life. Vertical cracks effectively adapted to the volume change of coatings during heating/cooling cycles, resulting in thermal fatigue life of TBCs increased significantly. Additionally, the uniformly distributed pores in the YSZ coating have a more significant effect on the thermal fatigue of the TBCs by reducing the elastic modulus of the coating. Park et al. [90] discussed the effect of substituting cerium for yttrium stabilizer on the thermal corrosion properties of TBCs from a microscopic point of view. The results showed that even within one hour of the thermal corrosion test, the penetrating salt was close to the interface of the bond-coat, and the reaction between the penetrating salt and the tetragonal stabilizer in zirconia occurred, with the transformation from tetragonal phase to monoclinic phase. Unexpected failures may occur under thermal shock conditions in corrosive environments, especially in YSZ-TBC systems [89]. Therefore, the failure caused by CMAS is closely related to the thickness of deposition and cracks. Cracks easily appear at the interface between the top layer and CMAS during cooling, the difference of thermal expansion coefficient leads to the generation of residual stress, which causes the failure of the coating. Additionally, the composition of the material, the thickness of the coating, and the defects in the coating will affect the high temperature corrosion rate of the hot-section components.

Figure 12. (a) Distribution of shear stress $\sigma_{12}$, stress in the $y$-axis direction $\sigma_{22}$, and max in-plane principal stress $\sigma_{\text{mp}}$ around the microstructure with and without CMAS at different cooling times, (b) magnification of zone I with CMAS and zone II without CMAS shown in (a). Reprinted with permission from [84]; Copyright 2019 Elsevier.
The traditional high-temperature resistant ceramic materials would not meet the existing needs. The development of a new generation of ultra-high temperature TBCs (working at different temperatures) is also urgent. However, due to the influence of ultra-high temperature, the current material processing equipment, and processing technology are also greatly limited.

4. Conclusions and Prospects

- The performance of the material is dependent on the microstructure of the material. The dual-ceramic coating has higher thermal insulation performance and can greatly prolong the thermal cycle life of the coating, improving the service temperature of the coating significantly. It is one of the effective ways to develop ultra-high temperature TBCs in the future.
- At present, the factors affecting the service lifetime of TBCs, such as TGO, thermal mismatch, and high temperature corrosion, are being studied. The damage of TBCs caused by CMAS at high temperature is emphasized. However, it should not be ignored that the uneven growth of TGO will cause the accumulation of residual stress and affect the distribution of interfacial stress. Additionally, the mechanism of the influence of the distribution of horizontal and vertical cracks on the stress around TGO during thermal cycling is revealed by finite element simulation. The thermal shock resistance of the coating can be further improved by controlling the density of the segmentation cracks.

With the development of space technology, the urgent need to achieve space-space integration has become the focus of development in the research and development of supersonic missiles, space rockets, and space shuttle vehicles. In the extreme environment of long-term hypersonic cruise, the severe friction between the wing and the atmosphere creates extremely high temperatures. Additionally, the engine intake is subjected to extremely high thermal loads and mechanical loads during flight. The traditional high-temperature resistant ceramic materials would not meet the existing needs. The development of a new generation of ultra-high temperature TBCs (working temperature above 1500 °C) is also urgent. However, due to the influence of ultra-high temperature, the current material processing equipment, and processing technology are also greatly limited.

How to design and prepare ultra-high temperature protective materials with good oxidation resistance, ablation resistance, thermal shock resistance, and maintain a certain ultra-high strength has become an essential technology to be solved urgently for new aircraft. In the complex ultra-high temperature service environment, due to the limitations of experimental conditions, there are few reports on the theoretical model of residual thermal stress experienced by ultra-high temperature ceramic coatings at different temperatures.
In addition, the effect of the change of CMAS erosion on hot-section components of aviation aircraft can be simulated by finite element calculations due to the change of CMAS corrosion. The concurrent mode of catastrophic failure caused by the deposition probability of inhaled particles and the relationship between different failures has not been fully studied. While the previous reports mainly focused on the simulation of TBCs residual stress during thermal spraying and actual service, the influence of cracks on the service lifetime of coatings should not be neglected.

Besides, how to reduce the experimental cost through simulation and optimize the process also faces great challenges, Liu et al. [91] simulated the preparation process of PS-PVD to produce TBC by the available finite element software ANSYS Fluent 16.0. The deposition quality of TBC was adjusted by altering the size of the free plasma jet, spraying distance, and feeding powder rate, which provide a basic method for further research on the transport of gas-phase materials for TBC in the boundary layer. However, the spraying environment pressure was considered to be constant at 100 Pa and the substrate temperature was constant at 1000 °C. PS-PVD is seriously affected by the track of environment pressure and temperature. Particles in the process of spraying are not taken into account in the actual environment, which may lead to local temperature change caused by collision and splashing, then affect the atmospheric pressure of the environment. In turn, the quality of the coating is affected, including the formation of pores and cracks. Therefore, further research will make an effort to optimize the preparation process of TBCs by simulation based on the working conditions.

At present, there are few studies on the lifetime prediction of TBCs. Therefore, under different application conditions, there is still much work to be done on the lifetime prediction of TBCs. In order to achieve this goal, the simulation of crack propagation is an important method and approach to predict the lifetime of TBCs.

Although the virtual crack closure technique (VCCT), extended finite element method (XFEM), and cohesive zone model (CZM) are used to solve the problems of crack propagation, simulation is limited when there are multiple branching or connecting cracks, as shown in Table 2. There are many random micro-pores and micro-cracks in TBCs. Crack growth in this kind of irregular structure is a very important research area. In addition, for the crack growth at the blade of the engine, the traditional way is to eliminate the residual stress generated by the crack by cold processing, such as shot peening, or to prevent the crack from appearing by adding TiO₂ and other substances at the crack. However, the occurrence of cracks is often accompanied by the release of energy. How to effectively control the cracks to spread in a favorable direction is also worth studying. There are no effective methods and procedures to solve these problems. Therefore, the heat transfer and failure of TBCs are still challenging issues which should be further investigated in the future.
Table 2. Comparison of VCCT, XFEM, and CZM.

<table>
<thead>
<tr>
<th>Methods of Computational Mechanic</th>
<th>Description of the Model</th>
<th>Advantages</th>
<th>Disadvantages</th>
<th>References Note</th>
</tr>
</thead>
<tbody>
<tr>
<td>Virtual Crack Closed Technique (VCCT)</td>
<td><img src="image1.png" alt="VCCT Diagram" /></td>
<td>★ It is extraordinarily suitable to count the energy release rate in the process of crack growth based on the thought that the energy required is equal to the work of marking the crack closed, when the crack propagates a tiny displacement.</td>
<td>◆ An initial crack should be predefined before the simulation of crack propagation</td>
<td>[37,92,93] Calculate $J$ integration</td>
</tr>
<tr>
<td>Extended Finite Element (XFEM)</td>
<td><img src="image2.png" alt="XFEM Diagram" /></td>
<td>▲ It is not essential to define an initial crack&lt;br&gt;▼ It can solve the problems of crack propagation with non-continuous characteristics&lt;br&gt;▲ The propagation path of the cracks is also not essential to be defined, not dependent on the inner details of geometrical structure only dependent on the external shape of the structure body</td>
<td>▼When the crack propagates to a complicated interface, it is not very effective to model the problems of the interfacial fracture</td>
<td>[94–97] Calculate propagation of the crack at the inner of the top coat</td>
</tr>
<tr>
<td>Cohesive Zone Model (CZM)</td>
<td><img src="image3.png" alt="CZM Diagram" /></td>
<td>▲ It can solve the problem of the energy dissipation based on the degradation of interface stiffness&lt;br&gt;▼ It is not essential to refine the mesh during the simulation process, and the crack is not necessary to be prefabricated</td>
<td>■ Many parameters should be set&lt;br&gt;■ The computational cost is high</td>
<td>[98–102] interfacial fracture</td>
</tr>
</tbody>
</table>
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Conflicts of Interest: We declare that we have no conflict of interest.

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