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Review article

Modeling of thermal properties and failure of thermal barrier coatings with the use of finite element methods: A review

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ABSTRACT

To understand the thermal insulation and failure problems of the thermal barrier coatings (TBCs) deeply is vital to evaluate the reliability and durability of the TBCs. Actually, experimental methods can not reflect the real case of the TBCs during its fabrication and service process. Finite element modeling (FEM) play an important role in studying these problems. Especially, FEM is very effective in calculating the thermal insulation and the fracture failure problems of the TBCs. In this paper, the research progress of the FEM on the study of the thermal insulation and associated failure problems of the TBCs has been reviewed. Firstly, from the aspect of the investigation of the heat insulation of the TBCs, the thermal analysis via FEM is widely used. The effective thermal conductivity, insulation temperature at different temperatures of the coating surface considering the thermal conduct, convection between the coating and the environment, heat radiation at high temperature and interfacial thermal resistance effect can be calculated by FEM. Secondly, the residual stress which is induced in the process of plasma spraying or caused by the thermal expansion coefficient mismatch between the coating and substrate and the temperature gradient variation under the actual service conditions can be also calculated via FEM. The solution method is based on the thermal–mechanical coupled technique. Thirdly, the failure problems of the TBCs under the actual service conditions can be calculated or simulated via FEM. The basic thought is using the fracture mechanic method. Previous investigation focused on the location of the maximum residual stress and try to find the possible failure positions of the TBCs, and to predict the possible failure modes of the TBCs. It belonged to static analysis. With the development of the FEM techniques, the virtual crack closure technique (VCCT), extended finite element method (XFEM) and cohesive zone model (CZM) have been used to simulate the crack propagation behavior of the TBCs. The failure patterns of the TBCs can be monitored timely and dynamically using these methods and the life prediction of the TBCs under the actual service conditions is expected to be realized eventually.

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1. Introduction

Thermal barrier coatings (TBCs) which are deposited onto the superalloy substrates are important ceramic coating materials. They are usually used for the parts of gas turbines, e.g., combustions chambers, turbine blades, or vanes, of an aircraft or of a power plate for generating electricity, steam turbine, or compressor. The TBCs are usually composed of metallic bond-coat and ceramic top-coat. The bond-coat is usually composed of MCrAlY (where M = Ni and/or Co), the ceramic top-coat is usually composed of 6–8 wt.% yttria stabilized zirconia (YSZ). Generally, the TBCs fabricated by atmospheric plasma spraying (APS–TBCs) has exhibited lamellar structural characteristic. Micro-pores and micro-cracks are distributed at random in the ceramic top-coat, the APS–TBCs usually has relatively low thermal conductivity. While the TBCs fabricated by electron beam–physical vapor deposition (EB–PVD) has typical characteristic with columnar grains. The adjacent columnar grains are leaned with each other. This kind of TBCs usually has high strain-tolerance and it is beneficial to improve the thermal shock resistance ability [1–8].

With the increasing of the working temperature of the hot-section components of turbine blades, the demand to the TBCs which are coated on the turbine blades is becoming higher and higher. The TBCs will play an more important role in controlling the gas with the high temperature eroding against the surface of the turbine blades (Fig. 1), and the coated TBCs will make the turbine blades work at higher temperature [9–12]. As the TBCs were usually applied at the extreme service conditions, the peeling phenomenon at early stage is inevitable. Microstructure is also not controllable. The service performance and the short lifespan are usually the disadvantages for the TBCs, so the TBCs with high performance under the actual service conditions is very important. To fabricate the TBCs with excellent performance from the experiment methods is very complicated and there are many unknown factors and should be further explored and persisted for long time. The computational simulation can help us optimize the fabrication technique and coating structure in the laboratory, save the investigation time and research cost and make the work has high efficiency. The computational simulation methods can help us find the optimized techniques and coating structure under the condition of the specific objective [13]. Before to design the TBCs with excellent performance, we should know the laminar structure, irregular microstructural characteristics and associated fabrication techniques of various kinds of TBCs. Fig. 2 shows the movement process of spray gun in the spraying process for the plasma-sprayed TBCs. The microstructure of the as-sprayed TBCs is also shown here, micro-pores and micro-cracks are distributed at random in the TBCs [14]. As the TBCs exhibit the duplex layer structural characteristic, it can be regarded as the laminar composite materials. The reliability and durability are the two important aspects for the TBCs. The reliability demand that the TBCs has high adhesive strength, high thermal insulation, low residual stress and high performance at high temperature. While the durability demand that the TBCs has high lifespan when they was used under the actual service conditions [15–18].

The distribution of the temperature field and residual stress are two important aspects for the TBCs when they were used under the actual service conditions. The effective thermal conductivity or heat insulation effect are usually calculated by the distribution of the temperature field, the FEM is very effective to calculate the distribution of the temperature field of the TBCs [19–24]. In fact, the microstructure of the as-sprayed TBCs is very complicated as well as the exterior service conditions, such as nonlinear temperature gradient, strong oxidation condition, CaO–MgO–Al_2O_3–SiO_2 (CMAS) impact erosion and so on [25–29]. When considering the intrinsic microstructural characteristic, heat conduction of the TBCs itself, the convection between the TBCs and the environment, heat radiation at high temperature, even the phonon scattering for the nanostructured TBCs, the effective thermal conductivity of the as-sprayed TBCs can be calculated in theory via FEM [30,31].

And the residual stress is also very important for the TBCs, it can affect the failure modes and lifespan of the as-sprayed TBCs. Many previous literatures have reported the distribution of the residual stress of the TBCs when they were subjected to different service conditions [32], and the residual stress of various types of the TBCs has been calculated by FEM. In fact, in the process of the fabrication, the residual stress can be induced in the TBCs. In addition, the residual stress can be also induced and developed when the TBCs were endured with the thermal shock, high temperature oxidation and other conditions. The FEM can calculate the residual stress of the TBCs effectively based on the thermal–mechanical coupling technique [33–42].

In fact, the previous report about the calculation of residual stress via FEM mostly stayed at static thinking perspective. The failure of the TBCs is usually caused by the crack nucleation, grow and propagate [43,44]. In the previous work, the failure modes and failure positions are often judged by the value and location of the maximum principal-stress. The crack propagation behavior was often predicted by the simulation results of the residual stress. Only the crack nucleation positions will be considered. How the crack will propagate was not taken into account. So this limitations promote new computational methods appear in order to solve these problems. With the development of FEM techniques, the FEM can also solve these problems based on the fracture-mechanic method. Usually, stress tend to concentrate at the crack tip, the stress intensity factor and energy release rate or *J*-integral can be calculated via FEM. The crack propagation path can be also further simulated based on the other techniques [45–52], such as virtual crack closured technique(VCCT), extended finite element method (XFEM) and cohesive zone model (CZM). The VVCT is a very important computational mechanic method to calculate the energy release rate of the propagated crack based on the thought that the necessary energy when the crack propagate a tiny displacement is equal to the work of making the crack closed. If there is a crack in the TBCs, whether the crack will propagate can be judged by the calculation of energy release rate using VCCT method. XFEM is a new FEM technique which has been developed and promoted in the past decades, especially, it has inherited the advantage of conventional FEM. It can solve the problems of crack propagation with non-continuous characteristics without defining an initial crack. And when the crack propagate a certain displacement, the model is not necessary to be remeshed. It can also trace the propagation of the crack and find out the position of the propagating crack. The XFEM can be used to simulate the propagation behavior of the cracks at the ceramic layer of the TBCs. While the cohesive zone model (CZM) can solve the problems of the energy dissipation based on the degradation of interface stiffness. It is not necessary to refine the mesh during the simulation process, and the crack is also not necessary to be pre-

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