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Finite element simulation of stress distribution and development in 8YSZ and double-ceramic-layer $La_2Zr_2O_7$/8YSZ thermal barrier coatings during thermal shock

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ABSTRACT

In this paper, the thermal stress of the double-ceramic-layer (DCL) $La_2Zr_2O_7$/8YSZ thermal barrier coatings (TBCs) fabricated by atmospheric plasma spraying (APS) during thermal shock has been calculated. The residual stress of the coating after being sprayed has been regarded as the initial condition of the first thermal cycle. The characteristic of the stress development during the thermal cycle has been discussed, and the influence of the defects on the failure mode during the thermal cycle has also been discussed systematically. Finite element simulation results show that there exist higher radial thermal shock stresses on the ceramic layer surface of these two coatings. There also exist higher thermal stress gradient at the interface between the ceramic layer and the metallic layer. Higher thermal stress in 8YSZ/NiCoCrAlY coating lead to the decrease of thermal shock property as compared to that of LZ/8YSZ/NiCoCrAlY coating. The addition of LZ ceramic layer can increase the insulation temperature, impede the oxygen transferring to the bond coating and can also reduce the thermal stress. Considering from the aspects of thermal insulation ability and the thermal shock resistance ability, DCL type LZ/8YSZ TBCs is a more promising coating material compared with the single-ceramic-layer (SCL) type 8YSZ TBCs for the application.

1. Introduction

As a very important ceramic coating, thermal barrier coatings (TBCs) play an important role in protecting the high temperature components (superalloy) from being thermal corrosion and wear, they are often considered or being used in the aircraft and turbine blades [1–7]. There are two common ways to fabricate the TBCs, i.e., atmospheric plasma spray (APS) [8–10], and electrical beam-physical vapor deposition (EB-PVD) [11–13]. The coating fabricated by APS often exhibits laminar structural characteristic. Pores and cracks are inevitable due to the internal thermal stress in the process of thermal spraying. While the coating fabricated by EB-PVD often exhibited columnar grain structural characteristic. During the past decades, many investigations are often focused on the following aspects: (1) the fabrication of feedstock and corresponding coating and their microstructual and mechanical properties characterization [14–21]; (2) the thermal insulation behavior of TBCs [22–25]; (3) the thermal shock and high temperature oxidation resistance ability of TBCs [26–32]; (4) failure mode at high temperature and the life prediction of TBCs [33–42]. With the development of the modem industry, the demand to the thermal barrier coatings with excellent performance is becoming more and more urgent. The durability of the coatings is becoming more and more important. The evaluation and prediction of lifetime for the TBCs is a hot problem for the researchers. Generally, it was well known that the lifetime and the durability of the TBCs are often determined by residual stress or thermal stress. When the coating endures the thermal cycles between the hot gas and cooling air, the thermal stress will be induced. It was necessary and important to evaluate and predict the development of the stress in the TBCs during thermal shock. Finite element method is an efficient method to characterize and predict the thermal stress in the TBCs. Zirconate-based thermal barrier coatings are expected to be the candidate materials for the future application in aircraft, turbine and other high temperature components due to its lower thermal conductivity, higher stability and higher sintering resistance ability at

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high temperature [43–47]. $La_2Zr_2O_7$ (LZ) is a typical representative. Although much literature reported the thermal physical properties of zirconate-based bulk materials, little was focused on the investigation of the zirconate-based TBCs. Some literatures have reported the thermal shock behavior of zirconate-based TBCs fabricated by EB-PVD [48,49]. Little investigation was focused on the simulation of thermal shock behavior of the DCL TBCs fabricated by APS. This paper will try to investigate the stress distribution and development of the double-ceramic-layer LZ/8YSZ TBCs during thermal shock using the finite element method. And at the same time, the influence of defects on the thermal shock behavior has also been discussed.

2. Simulation procedures

In order to further investigate the failure mode of the nanostructured SCL 8YSZ TBC and DCL $La_2Zr_2O_7$/8YSZ TBCs, finite element simulation was performed. The commercial available ANSYS software (affiliated with APDL code) was used in the simulation [50]. The two models based on the structure of the SCL 8YSZ and the DCL $La_2Zr_2O_7$/8YSZ coatings were established. The thickness of the substrate, bond-coating and top-coating for the SCL 8YSZ TBCs are 6 mm, 100 μm and 300 μm, respectively. The thickness of the substrate, bond-coat, 8YSZ layer and the $La_2Zr_2O_7$ for the DCL $La_2Zr_2O_7$/8YSZ TBCs are 6 mm, 100 μm, 240 μm and 60 μm, respectively. In the present finite element analysis, the following assumptions were made: (1) the materials properties of $La_2Zr_2O_7$ and 8YSZ coatings were considered to be linear elastic, while elastic–plastic responses were included in both the substrate and bond coating; Von-Mises yield criterion and bilinear kinematic hardening were assumed to describe the strain-hardening behavior of substrate and bond coating; (2) although the coating property is different at the spray direction and the interface direction, the micro-defects, such as pores, cracks have no evident direction and the arrangement is irregular, the coating microstructure is not uniform. So the mechanical properties at different directions have little difference, the coating can be viewed as isotropic. The substrates were also isotropic due to that it was polycrystalline material. All the materials were temperature-independent; (3) the creep and oxidation behavior were not included in the models but will be further studied in the following paper.

Fig. 1 shows the model in the finite element simulation. The model was reduced to axisymmetric model in order to save the computational time. The right edge of the substrate/bond-coat interface, bond-coat/8YSZ interface, and 8YSZ/LZ interface are defined as Node A, Node B and Node C, respectively. As the stress at these interface edges has an interfacial edge stress singularity and the corresponding values are mesh dependent. The mesh around the edge is fine enough in the finite element simulation. Generally, the dense of the mesh, the accuracy of the solution result, but when the mesh is too dense, the solution time will be very longer, i.e., the solution efficiency will decline. So there is a proper mesh density when the solution efficiency and solution accuracy has a best match. A mesh design has been given in order to obtain the suitable value about the stress of Node A, Node B and Node C. In the finite element simulation, when the nodal value solution and element value solution of the whole thermal barrier coating system have the same order of magnitude, and the relative error is tiny, then the solution obtained from the finite element model with enough element number can be acceptable. The mesh of the model without defects and with defects can be seen in Fig. 2. In the present investigation, firstly, thermal cycle simulation for the coatings without defects was performed. In this section, the stress distribution and stress development during the thermal cycle will be discussed in detail.

Fig. 3 shows the flow chart of the simulation procedure of the thermal shock cycle, the simulation procedure can be described as follows:

Step 1: Select the element properly, the model was established suitably, and the corresponding material parameters have been assigned to the model (Table 1), making the mesh to the model, all the initial temperature conditions and structural boundary conditions were imposed on the model. All the elements were killed except the substrate elements before the first time calculation.
Step 2: Active the first layer elements from the bottom, and perform the first time calculation, when the calculation was completed successfully, active the second layer elements and perform the second time calculation. Perform all the calculation till all the elements of the model were activated.
Step 3: When the coating has been deposited, the finished state in the Step 2 was regarded as the initial state of this step (including the temperature and stress distribution). The whole coating system has been cooled to ambient temperature from the high temperature, and perform the residual stress calculation after thermal spraying.
Step 4: When the Step 3 was finished, the stress can be regards as the initial condition of the first thermal cycle, and perform the stress calculation of the first thermal cycle.
Step 5: When the calculation of the first thermal cycle has been finished, the residual stress after the first thermal cycle was regarded as the initial condition of the second thermal cycle, and performs the calculation of residual stress of the second cycle. Repeat the similar process till all the cycles which are assigned are finished.

In our present study, the whole process that the model was "heated" to 1200 °C in the muffle furnace with a dwell time 5 min, and then quenching into the water was regarded as a thermal cycle.

3. Results and discussion

In this section, the simulation results about the stress development and distribution during the thermal cycle have been extracted from the ANSYS visualization and analyzed systematically. Residual stress components resulting from the finite element analysis were obtained in the following directions: (1) radial stress corresponding to stress value along the radial direction (σ_{xx}); (2) axial stress component that refers to stress profile through the thickness of coatings (σ_{yy}) and (3) shear stress component that acts along the tangential direction (σ_{xy}).

3.1. Stress development and distribution in the TBCs during thermal shock

Fig. 4 shows the distribution of residual stress of σ_{xx}, σ_{yy} and σ_{xy} after the LZ/8YSZ TBCs being cooled to the ambient temperature (100 μm NiCoCrAlY bond-coat, 240 μm 8YSZ ceramic-coat and 60 μm LZ top-layer). It can be seen that the maximum radial tensile stress is located at the LZ layer surface, the maximum radial compressive stress is located at the NiCoCrAlY/substrate interface and near the right edge of the coating system (Fig. 4a). The maximum axial tensile stress is under the edge below the NiCoCrAlY layer. The maximum axial compressive stress is located at the edge of the center of the substrate (Fig. 4b). The maximum shear tensile stress is located at the substrate and near the right edge, and stress which is located at the 8YSZ layer edge is near the maximum stress magnitude, but the maximum shear stress is only 32.1 MPa, this value is low and usually cannot make a crack to initiate. The maximum compressive axial stress is located at the NiCoCrAlY/substrate interface and near the right edge (Fig. 4c).