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Finite element simulation of residual stress and failure mechanism in plasma sprayed thermal barrier coatings using actual microstructure as the representative volume

N. Nayebpashaee [a,*], S.H. Seyedein [a], M.R. Aboutalebi [a], H. Sarpoolaky [b], S.M.M. Hadavi [c]

[a] Materials Processing Simulation Laboratory (MPS-LAB), School of Materials and Metallurgical Engineering, Iran University of Science and Technology (IUST), Narmak, Tehran, Iran
[b] School of Materials and Metallurgical Engineering, Iran University of Science and Technology (IUST), Narmak, Tehran, Iran
[c] Research Department of Ceramics, Materials and Energy Research Center (MERC), Karaj, Iran

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ABSTRACT

The residual stress and failure mode of thermal barrier coating (TBC) containing metallic bond coat (BC) and ceramic top coat (TC) with and without thermally grown oxide (TGO) were predicted using a micromechanical-based finite element method (FEM). Actual microstructures of the TBC taken by a scanning electron microscope (SEM) were utilized as the representative volume elements (RVEs) in the computational model. Failure mode of the representative volume was numerically simulated as thermal stress localization during thermal cycle. Computations were done on the representative volume to quantitatively assess the effects of thermal and mechanical properties of the TBC constituents as well as the presence of TGO on the macroscopic mechanical response of the TBC. Comparisons of computed results with experiments verified that, the computational method can successfully predict residual stress and crack initiation mode of the studied thermal barrier coatings. Moreover, based on the computed results, both shear and normal failure mode occur in the thermal barrier coating which is in good agreement with experimental findings.

1. Introduction

Thermal barrier coatings (TBCs) are one of the most conventionally-used protective materials which are employed as insulation media to save underlying metallic substrate from harmful effects at high temperature services [1]. A typical TBC is composed of two layers including the bond coat and top coat. The bond coat with metallic structure has the chemical composition of MCrAlY (where M = Ni and/or Co) and the ceramic-based top-coat is often made of yttria stabilized zirconia (YSZ) or cerium stablized zirconia (CSZ) [1].

Problems such as phase transformation, volume shrinkage stemmed from sintering and even, increasing elastic modulus limit the operating temperature of such materials to a maximum of 1473 K for long-term use and this is the main drawback of YSZ. To find a solution for this, the search for new materials has been widely done in recent years and since then, hybrid lanthanum zirconate-based TBCs are considred to be a high-quality candidates for the future application in high temperature applications. Low thermal conductivity, high stability and resistance to sintering at high temperatures which avoid air void closure at mentioned limiting temperatures are some of the outstanding standpoints of this modern materials. $La_2Zr_2O_7$ (LZ) is one of the nominee materials and so far, little investigation was focused on the thermal shock behavior of the double-ceramic-layer (DCL) TBCs [2–3].

All constituents in a TBC system including substrate and BC with metallic characteristics and ceramic-based TC have noticeably different physical and thermo-mechanical properties, especially when temperature dependency and thermal shock is taken into account, which made understanding, simulation and further interpretation of problem over-detailed and complicated [4]. Residual stresses developed in TBC systems are usually due to the following events in real conditions: stresses induced during phase transformation, solidification and subsequent contraction of splat droplets from spraying temperature to the room temperature and stresses caused by the difference between the linear coefficients of thermal expansion (CTE) in different layers. This matter get much disastrous and catastrophic when system cools down from much higher temperatures to the ambient temperatures which significantly decrease the lifetime of protective layer and need underestimated overhaul [5].

It has been pointed out in various researches that, after fabricating thermal barrier coatings using thermal spray technique, a rough interface is left after sand blasting procedure [6]. This micron-size rough interface formed between layers has relatively positive and negative effects. In positive view, layer adhesion enhanced because of mechanical inter-locking and this can considerably rise to the lifetime service of a plasma-sprayed coating system by stopping delaminating and also spallation in interlayer regions. In the counter point of view, curved and rough boundary line between layers can act as potential

* Corresponding author at: School of Materials Science and Engineering, Iran University of Science and Technology (IUST), Narmak, Tehran, Iran.
E-mail address: Nayebpashaee@iust.ac.ir (N. Nayebpashaee).

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to non-uniform stress distribution and strain localization that can consequently cause more potent crack initiation zones [7].

One of the predictable phenomena usually takes place in TBC systems and in some cases known as the main failure factor of system is the growth of thermally growth oxides (TGO) with different thicknesses and morphologies that have been taken into consideration in many studies [8–9]. At higher temperatures in the interface of BC/TC, diffusion is dominant because of its thermally activated nature and causes simultaneous outward and inward migrations of aluminum and oxygen, respectively. This reverse movement of aluminum and oxygen atoms led to the formation of aluminum oxide compound layer and usually limits the efficiency of the coating. The resistance to free expansion and contraction caused by the presence of TGO induces residual stress in interlayer regions and makes the system persuasive to fracture and fatigue crack growth [10]. This is a major failure mechanism developed at the interface formed as a result of bond coat oxidation at about 900 ºC. The effect of formation of this oxide layer has been the subject of different investigations in which several parametric studies were done considering alumina oxide layer, interface shape morphology and non-homogeneity of thermal loading [5,10–11].

Another foremost limitation in this high temperature protective system is the interfaces between substrate/BC and BC/TC. These interface regions undergo high stress concentration due to the mismatch of thermal expansion between materials and due to interface roughness which is another main reason of failure and fracture in TBC systems [12–13].

There are many researches about fracture mechanic approach, stress state evolution and failure mechanism of thermal barrier coatings using both analytical and numerical methods. Some of these investigations incorporate the molecular dynamic (MD) model to study phase transition behavior of YSZ materials [14], finite difference method (FDM) [15] for thermal conductivity change modeling and the finite element method (FEM) for multi purposes [4–5,11,16–18]. Among these modeling approaches, FEM has this advantage to use real microstructure as calculation domain [19–22] and presents maximum similarity to the actual conditions in material structure.

In the prediction of stress distribution by micromechanical finite element methods [23–25], in which real microstructure of multilayer thermal barrier coating utilized as a representative volume, no prearrangement and mathematical failure norm need to be implemented and stress amplification and recognition of crack initiation are recognized as the natural conclusion of the stress concentration and localization due to the incompatible contraction between the ceramic and metallic layers. According to the literature [17–18,26–27], none of the other simulation models for predicting stress distribution of multilayer thermal barrier coating have this unique outstanding facility, which causes the application of micromechanical model to be common, applied and quite efficient.

In the mentioned papers which used FEM, temperature distribution as well as thermally induced stresses, crack propagation and failure modes of ceramic thermal barrier coatings have been numerically investigated practically. However, none of the performed modeling techniques for simulating the thermomechanical response of TBCs have such a remarkably excellent characteristic, which use RVE-based micromechanics to be common, useful and quite straightforward.

The purpose of the current study is to predict the temperature distribution and induced residual stress in TBCs with and without TGO using finite element method, in which the real microstructure of the sprayed coating was implemented as the representative volume elements. In all related researches found in the literature, the mechanical properties of each layer of the multi-layer media have been determined using the measuring experimental method while in this work, the mechanical properties of all materials used in TBC have been used based on the experimental results reported in the literature.

2. Experimental procedure

In this research, micron size yttria stabilized zirconia (YSZ) with powders in size range of 15–106 μm, as seen in Fig. 1, (commercial code: Metco 204NS-G) was used to prepare a thermal barrier coating on the cast INCONEL 738 Nickel-based superalloy.

This point has to be taken into consideration that, all mathematical descriptions and results achieved and discussed here are applicable for TBC system with micron-size YSZ top coat but not nano-agglomerated nor nano-size ingredients. As mentioned in many studies [28–30], nano-size powders and coatings possess relatively different characteristics and performances comparing to conventional YSZ and were not considered in this paper.

Initial powders were heat treated for 2 h at 100 °C for removing the humidity just before spraying to the substrate surface and in addition, for a better substrate roughness and also clean surface, INCONEL was blasted with silicon carbide particles with a mesh number of 24 in. with an optimum pressure of 4.5 bars followed by smooth grinding, degreasing and acid pickling. It is noted that, bond coat with chemical formula of $Ni_{22}Cr_{10}Al_1Y$ (commercial code: AMDRY 962) and particle size of about 45–130 μm were deposited just before having YSZ sprayed. Both metallic bond coat and ceramic heat resistive top coat were put down on the Nickel-based alloy using a plasma spray apparatus with water cooled gun Type 3 MB of MTECO company. Plasma spraying parameters used for TBC coating are listed in Table 1. For evaluation of materials formed in the upper surface of the coating, an X-ray diffraction analysis was done to characterize the coating surface after cooling down of as-sprayed sample using a Siemens D 500 apparatus. For performing thermal shock, two routes were considered; one without dwell time and another with 300 s of temperature soaking at 1300 °C. However, in both cases, the samples were heated up to target temperature of 1300 °C from air in electrical furnace followed by an air cooling to 25 °C via an air jet apparatus. It should be added that, both thermal shock regimes i.e. with oxidation time (cause of TGO formation) and without it (no TGO) were repeated for 45 times. At last for revealing the microstructure of multiple-shocked coatings in SEM studies, samples were mounted, grounded and polished.

3. Finite element analysis

Hypothetically, the macroscopic manners of thermal barrier coating systems can be numerically modeled from its atoms, lattice, grain structure, and microstructure up to the macroscopic constitutive order. In spite of the fact that material extrinsic constitutive modeling is the best and most efficient option for numerical modeling and subsequent simulation of phenomena, it usually offers no sensitive data about stress distribution mode and failure mode in the studied materials. In this research, thermo-physical and mechanical properties of each of the TBC layers have been considered to be temperature-dependent and isotropic in order to simulate the temperature distribution, residual stress and potent zones to crack initiation with FEM numerical approach. Fig. 2 illustrates the scanning electron micrograph (SEM) from the as sprayed and shocked thermal barrier coating on as-cast INCONEL 738 alloy with and without thermally grown oxide. It is worth reminding that, micrograph 2.b has experienced a dwell time at high temperature in addition to heating and cooling regime that used for both. The difference in brightness through SEM micrographs shows different layers of substrate, metallic bond coat, TGO and ceramic top coat.

TBC system considered in this research is the high temperature protective layer used in the hot-section of a gas turbine with the approximate geometry as indicated in Fig. 3a. Fig. 3a, b and c show the main body of coated part in a gas turbine, cross section and the final calculation geometry, respectively. Four independent variables of stress $\sigma = F(x, y, z, t)$ describe the process of thermal distortion in the TBC in which x, y, z are positions in Cartesian coordinate system and t is the