Surface & Coatings Technology 276 (2015) 399–407

Contents lists available at ScienceDirect

Surface & Coatings Technology

journal homepage: www.elsevier.com/locate/surfcoat

Multi-scale modeling of damage development in a thermal barrier coating

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ARTICLE INFO

Article history:
Received 10 February 2015
Revised 11 June 2015
Accepted in revised form 18 June 2015
Available online 19 June 2015

Keywords:
Thermal barrier coating
Thermally grown oxide
Top coat
Damage
Multi-scale numerical model
Roughness

ABSTRACT

A multi-scale Finite Element Microstructure MEshfree (FEMME) fracture model for quasi-brittle materials with complex microstructures is applied to simulate thermo-mechanical damage in a plasma-sprayed thermal barrier coating system. This novel multi-scale technique for damage simulation allows the influence of the microstructure of the yttria-stabilized zirconia top coat and the geometry of the bond coat and the thermally grown oxide layer to be considered with computational efficiency. Mechanical damage, due to the thermal strain of an applied temperature difference, is predicted to decrease the top coat Young's modulus. The interaction between the evolution of damage and temperatures within the top coat is also simulated, demonstrating the capability of this methodology to address coupled multi-scale problems.

1. Introduction

Thermal barrier coatings (TBCs) are multilayer coating systems used in propulsion and power generation industries to protect critical engineering components, such as burner liners, combustion chambers, vane platforms and turbine blades, against high-temperature oxidation and hot-corrosion. The TBC also lowers the substrate surface temperature, allowing improved service lifetime of the component and increased engine efficiency [1–5]. A typical TBC consists of: (i) an aluminum-rich metallic bond coat (BC), often MCrAlY-type where M is Co, Ni, or a combination of both; (ii) a thermally grown oxide (TGO) layer that forms during high-temperature exposure and (iii) a ceramic top coat (TC) of yttria-partially-stabilized zirconia (YSZ, i.e. $ZrO_2 + 6–8$ wt.% Y_2O_3) that provides thermal insulation.

Plasma spraying is a well-established process for TBC deposition, offering high deposition rates and low production costs. The microstructure of plasma-sprayed coatings features a lamellar structure of flattened 'splats' formed when molten particles solidify upon impact, randomly distributed pores, longitudinal 'intersplat' and short traverse 'intrasplat' microcracks that arise from quenching stresses (i.e. tensile stresses generated by shrinkage of the molten splats [6]) and a very small fraction of partially non-melted powder that arises from variations in temperature and particle velocity during spraying [7–10]. The microstructure is thus significantly affected by the process conditions, which include powder morphology and size-distribution, the deposition conditions (plasma power, gas composition and flow, powder feed rate, stand-off distance, spray angle, etc.) and geometrical factors (e.g. curvature and roughness of the interfaces of the substrate and the BC). The versatility of plasma-spraying permits the coating properties to be tailored for specific applications [10–15].

The failure of plasma-sprayed TBCs is affected by the microstructure and the thermal exposure history. Failure is generally connected to the evolution of the TGO layer, and occurs by propagation and linking of multiple cracks prior to spallation of the TC. For instance, delamination cracks propagate within the TC or TGO after initiation at imperfections in the vicinity of the irregular TC/BC interface [1,4,15,16]. The delamination path depends on the thermal exposure mode: isothermal oxidation promotes crack propagation within the TGO while thermal cycling leads to damage within the TC. Thermal low-cycle fatigue crack growth is driven by thermal strains resulting from high thermal expansion mismatch.

The geometry of the TC/BC interface influences the evolution of the stresses in the TBCs during thermal exposure [47], and may therefore be a significant factor in damage development. Recent experimental results show that modification of interfacial roughness, which can be done by varying the spraying conditions [17] or dry-ice blasting [18], is a promising route to lifetime improvement, yet the precise mechanisms and the upper roughness limit for optimum performance remain unclear. Besides the thermal history, structure and geometry of the

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http://dx.doi.org/10.1016/j.surfcoat.2015.06.038
0257-8972/

coating, various other interrelated processes can influence damage development: these are most notably the inter-diffusion of various elements between the substrate, BC and TC, including segregation of impurities at the TC/BC interface as well as the gradual depletion of aluminum and other oxide formers from the BC [2,19,20]; the formation of less-protective undesirable oxides and spinels along the TC/BC interface [9]; and sintering and microcracking within the TC [21–23].

Given this degree of complexity, computational numerical models are important tools to aid the design of TBCs (e.g. [24–27]). For example, Busso et al. [24] simulated the stresses along a non-planar TC/BC interface (described by a cosine function); their finite element model (FEM) took into account the growth of the TGO layer, creep of the BC and the TGO layer and also elastic anisotropy and sintering of the TC, which was produced by Electron Beam Physical Vapor Deposition (EBPVD). Their simulation showed how the stresses within the TC and tensile tractions at the TGO interfaces develop during oxidation and upon subsequent cooling and how they are affected by the roughness, the creep strength of the BC and by the ratio of the in-plane/out-of-plane stiffness of the TC. A subsequent study by the same authors [25] focused on the role of fast-growing non-alumina oxides during the 'breakaway stage' of the BC oxidation. Ranjbar-Far et al. [46] analyzed, using a 2D multilayer FEM, the influence of the interface roughness and the material properties in the stress distribution of the TBC.

The models used in such simulations are very sophisticated and include many important material properties, but it is common to treat the TBC as a homogeneous defect-free continuum, and this may overestimate the effects of some individual variables. For instance, the propagation of a single crack along the TC/TGO interface has been addressed numerically [26] taking into account the TGO layer growth and creep deformation of all constituents. However, only minor differences were predicted for the stress fields from single and multiple thermal cycles, in contrast to the significantly different behaviors that have been observed experimentally [16]. This suggests that damage processes are not fully described by simplified models that do not consider the heterogeneity of the microstructure.

Although it is possible to set-up a conventional FEM of a TBC containing multiple microstructural defects (e.g. [28,29]), the required discretization imposes severe computational costs; it is for this reason that most models treat the TBC as a continuum. Such limitations hinder the development of reliable life prediction methods, which need to also account for complex and realistic operating conditions such as mixed mode thermal-oxidation/thermal-cycling exposure. The purpose of the work presented in this paper is to demonstrate a novel computational approach; a Finite Element Microstructure MEshfree (FEMME) fracture model that significantly reduces the computational burden while maintaining a high fidelity description of the microstructure and TBC geometry. We suggest that this multi-scale modeling approach can improve the efficiency of simulation of microstructure effects on TBC component performance. Here it is demonstrated in an examination of the potential effect of the roughness of the TGO layer on damage development in a coated tube. The numerical model is first presented and then applied to simulate the degradation of a thermal barrier coating across which there is an imposed temperature difference.

2. Numerical model

The FEMME [29,30] (Finite Element Microstructure MEshfree) method allows one to describe a complex graded microstructure, using a Cellular Automata (CA) model, with a generic FEM (Finite Element Model with irregular tetrahedrons) to simulate complex sample geometries, with computational efficiency. A general CAFE (Cellular Automata Finite Element) method with hexahedron FE elements and a microstructure formed by one phase with variable material properties was first presented by Shterenlikht and Howards [31], achieving successful results in the modeling of the fracture of steel. Following that methodology, in order to model quasi-brittle fracture in materials with a complex microstructure, we insert variations in its discretization and the relationship between the CA and FE (Finite Element) layers through the introduction of a Meshfree framework as further layer between them. The versatility of the Meshfree framework allows us to connect variable domains with different geometries and numbers of nodes. For this we enforce the maximum entropy conditions described by Arroyo and Ortiz [32] and the geometrical adaptive conditions of Saucedo-Mora [33]. Each layer defines a different size scale and is solved with a different method. For the large size scale macromechanical layer a standard, relatively coarse, finite element model is used. In the small size scale layer we use a cellular automata method, where the different cells represent the properties of the material. A Microstructural Adaptive Meshfree (MAM) framework has been developed to solve the displacements of the microstructural features in the intermediate layer. The Meshfree model uses the microstructural features as its discretization, dividing the microstructure into Particle Domains (PD) that represent each particle with a single domain, and Inter Particle Domains (IPD) that link the particles and represent the matrix. From the large scale downwards to the small scale the information is shared between layers by the displacements, which provide the boundary conditions. From the small scale upwards to the larger scale the information is shared by the energy homogenization of the damage in the material to link the effects of the eroded (i.e. damaged) cells of the CA with the FE behavior [34].

The FE part of the FEMME model is implemented, for convenience, within the software ABAQUS using C3D4 tetrahedral elements. We use a variation of the cohesive element, but instead of following a predefined cohesive law, energy homogenization provides information from the microstructure of the energy that is released by the damage (i.e. fracture) that occurs in the FE layer. This updates the mechanical response of the element. This process is described in detail in the following section.

2.1. Coupled thermal–mechanical model for thermal barrier coatings

Previous applications of the FEMME fracture model considered only the response to mechanical loading [30,35,37]. Here, the numerical model aims to reproduce the mechanical behavior of the TBC under the application of a thermal gradient. Microstructural damage affects thermal properties, so this coupled model combines the fracture model with a thermal model, implementing the interaction between them. In this way, thermal strains can introduce damage, and damage affects also the thermal conductivity and hence also the temperature distribution within the damaged material. The thermal model is introduced in the FE layer using the tetrahedral element with a single integration point C3D4T (i.e. a thermo-mechanical version of the element C3D4). The thermal model is introduced to the Meshfree model using Eq. (1),

$$\begin{matrix} K & C \\ 0 & D \end{matrix} \; \begin{matrix} U \\ T \end{matrix} = \begin{matrix} F \\ 0 \end{matrix} \qquad (1)$$

where K is the stiffness matrix of the static mechanical problem, D is the conductivity matrix of the thermal problem, and C is the matrix that introduces the thermal strains into the mechanical problem. The variables to be solved are the displacements U and the temperature T of each node of the discretization. Finally, F is the force vector applied to the system, which arises from the boundary conditions. As a simplification, we have only considered a steady temperature and the direct influence of the displacement field on the temperature has been neglected. This U–T relationship does exist indirectly through the effects of fracture, which is caused by thermal deformations and alters the conductivity of the damaged zones.

Fig. 1 shows a simple 3D elastic example of the method, developed here with large strains in order to enhance the contrast between compression and tension. The fictitious porous material has arbitrary