Computational Materials Science 116 (2016) 82–95

Contents lists available at ScienceDirect

Computational Materials Science

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

A computational framework for the interplay between delamination and wrinkling in functionally graded thermal barrier coatings

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ARTICLE INFO

Article history:
Received 28 June 2015
Accepted 16 August 2015
Available online 9 October 2015

Keywords:
Nonlinear finite element method
Nonlinear fracture mechanics
Wrinkling instability
Thin films
Functionally Graded Materials

ABSTRACT

Stiff films bonded to compliant substrates are used in a wide range of technological applications and especially in thermal barrier coatings (TBC). Thin films can be made of Functionally Graded Materials (FGMs) with a heterogeneous composition that usually range from a metallic to a ceramic phase. Aiming at investigating the phenomenon of delamination of thin FGM layers from compressed elastic substrates, a fully 3D nonlinear computational framework combining nonlinear fracture mechanics based on a novel interface element formulation for large displacements and a solid shell finite element to model the thin film is proposed. A comprehensive numerical analysis of delamination in TBCs is carried out, paying a special attention to the interplay between fracture and wrinkling instabilities. Results of the computations are also compared with benchmark 2D semi-analytical results, showing good accuracy of the proposed method that can be applied to general 3D configurations that are difficult to address by semi-analytical approaches.

1. Introduction

Thermal barrier coatings (TBCs) consisting of ceramic materials with a homogeneous composition are employed in a wide range of aerospace applications and in gas turbine technologies, among other engineering sectors. These coatings to protect the substrate from much higher temperatures than those admissible for uncoated systems. In this way, the temperature in the bulk is kept low thanks to the low thermal conductivity of the ceramic layer, sometimes coupled with active cooling of the metallic substrate. These systems are generally composed by an Aluminum-rich metallic bond coat (BC), providing protection against hot-corrosion and oxidation, and an outer ceramic top coat (TC) providing thermal insulation. As the ceramic layer is permeable to Oxygen, an inner oxide layer, the so-called thermally grown oxide (TGO), gradually evolves at the BC/TC interface during exposure to high temperatures.

A closer look at the interfacial zone actually shows that the BC/TC interface is not planar, see a collection of images taken from various sources in Fig. 1. Preliminary attempts to model this lack of planarity, considered as essential to accurately predict the stress field in the interfacial zone, have regarded FE stress analyses by approximating the interface waviness via sinusoidal functions [1], while a more accurate investigation of the lower scale random roughness has recently been proposed in [2].

Failure of TBCs and in general of very thin stiff coatings joined to a softer substrate is a complex mechanical phenomenon that involves a series of possible scenarios. This failure mechanism has been comprehensively investigated using semi-analytical [3,4] and numerical methods [5], being those applied to a wide range of materials and engineering problems. Considering a system predominantly compressed, wrinkle instabilities can take place when the bi-material interface possesses a strong fracture toughness, see Fig. 2(a). In other cases, buckling instabilities of the coating can take place, leading to interface delamination, see Fig. 2(b). Presumably, in the most general case, failure is a combination of these two individual mechanisms leading to wrinkles and buckling delamination at the same time, see Fig. 2(c).

Therefore, from the mechanical point of view, failure of layered systems can be investigated as the interaction between two elementary forms of nonlinearity, that is, buckling (geometrical nonlinearity) and fracture mechanics (mechanical nonlinearity).

Buckle delamination in 2D TBCs has been analytically studied in [7] as an interplay between linear elastic fracture mechanics and buckling. These forms of instabilities are certainly promoted by

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http://dx.doi.org/10.1016/j.commatsci.2015.08.031
0927-0256/

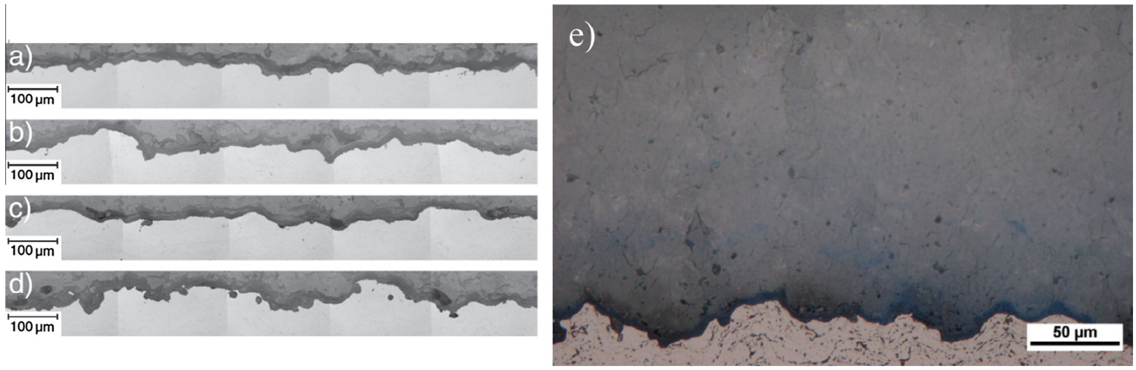

Fig. 1. Scanning electron and optical microscope images showing waviness and roughness of TBCs: (a–d) atmospheric-plasma-sprayed CoNiCrAlY + YSZ TBCs (adapted from [6]); and (e) roughness of the oxide layer consisting of Alumina with dispersed Y-rich oxides (adapted from [2]).

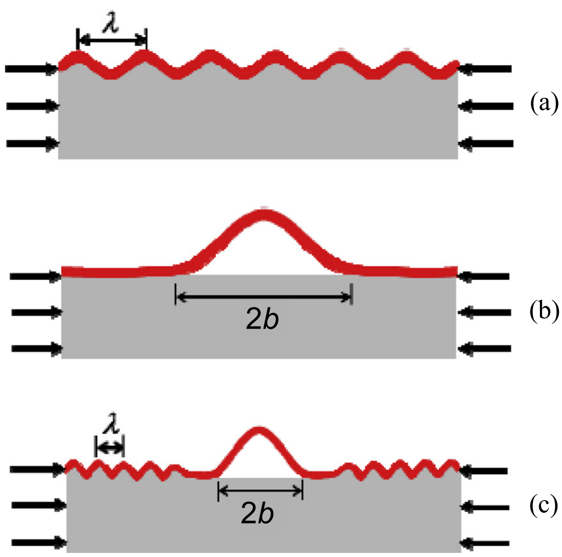

Fig. 2. Possible failure modes for a system with a stiff coating bonded to a softer substrate (adapted from [5]): (a) surface wrinkling with no delamination; (b) buckle-delamination; and (c) concomitant wrinkling and buckle–delamination.

the initial perturbations of the flat geometry due to waviness and roughness of the TGO. Fracture and delamination of TBCs has received a great deal of attention in the literature, since TBC durability relies on the integrity of the material interfaces [3,8–11]. Documented examples of fracture at the microscale are shown in Fig. 3, where crack nucleation often takes place at the BC/TC interface due to high residual stresses induced by a mismatch in the thermal expansion coefficients of the joined materials. Very recently, experimental evidence of geometrical instabilities has also been reported in elasto-plastic metal matrix composite layered micro-pillars under compression, under the form of wrinkles of the layers [12].

In the present study we propose an implicit finite element-based computational framework for the simulation of failure modes in three-dimensional functionally graded TBCs, accounting for both geometrical and material nonlinearities. The developed methodology comprises: (i) a large deformation solid shell finite element for Functionally Graded Materials (FGMs) [14], which is based on the formulation proposed in [15] incorporating the use of the Enhanced Assumed Strain (EAS) [16] and Assumed Natural Strain (ANS) [17] methods to prevent locking deficiencies, and (ii) a 3D nonlinear interface cohesive finite element to model delamination events undergoing geometric nonlinear effects.

The outline of the paper is as follows. Section 2 introduces the theoretical basis of the mechanical models for the thin layer and for the cohesive interface. Particularly, in Section 2.1 the basic solid shell finite element formulation in the total Lagrangian setting accounting for grading in the elastic properties of the TBC along its thickness is addressed. To simulate nonlinear cohesive fracture at the BC/TC interface, a large displacement interface element formulation allowing for displacement discontinuities at the interface is proposed in Section 2.3. It is noticed that the kinematic description of this interface element is fully consistent with that of the solid shell element, thus avoiding approximations required in the case of the use of alternative shell formulations based on rotational degrees of freedom. Section 3 presents the variational basis and the finite element (FE) formulation of both element topologies, which were implemented in the FE softwares FEAP [18] and ABAQUS [19] by the present authors. Section 4 focuses on the application of the proposed computational method, aiming at simulating the interplay between buckling and delamination in TBCs bonded to soft substrates. The results of the computations are compared with the analytical and numerical predictions presented in [5]. Finally, the main conclusions of this work are discussed in Section 5.

2. Fundamental equations

2.1. The structural thin film model

This section briefly outlines the fundamental aspects of the structural model used for the thin film, which is bonded to the homogeneous substrate. The present formulation finds its theoretical and computational basis in the finite kinematics shell presented in [20], which allows the use of three-dimensional material laws. Differing from the original formulation, where the continuum body parametrization is described in terms of its mid-surface, an alternative description relying on the solid shell concept is employed henceforth.

2.1.1. Kinematic description

Consider a shell body occupying a region in the Euclidean space $\mathscr{B}_0$ in the reference configuration. The position vector of a material point in the undeformed configuration $\mathbf{X}(\xi^1,\xi^2,\xi^3)$ is parametrized in the convective space $\xi = \{\xi^1,\xi^2,\xi^3\}$, with $(\xi^1,\xi^2,\xi^3) \in: \square = [-1,1]\times[-1,1]\times[-1,1]$, where $\square$ represents the unit cube, see Fig. 4. As customary in shell formulations, the coordinates ξ^1,ξ^2 are referred to the in-plane directions and $\xi^3 \in [-H/2, H/2]$ identifies the thickness direction, H being the initial shell thickness. The covariant basis vectors referred to the reference surface $\mathbf{A}_\alpha$ and to