Discrete Element Method to simulate interface delamination and fracture of plasma-sprayed thermal barrier coating (PARTICLES 2021)

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ABSTRACT

Thermal Barrier Coatings (TBC) are ceramic layers enabling metallic components to resist to severe operating temperature and prolonging their lifetime. Typically, TBC are composed of a ceramic Top-Coat (TC) for thermal insulation, an intermediate metallic Bond-Coat (BC) layer located between a superalloy substrate and the TC, and an oxidation-resistant layer called Thermally Grown Oxide (TGO). Predicting interface delamination and failure of TBC under thermo-mechanical loading is quite complex due to the severity of thermal conditions and the heterogeneity of their structure [1,2]. Besides, several parameters and phenomena lead to premature TBC failure reducing consequently their operating lifetime. Among these factors, thermal expansion mismatch, oxidation, interface roughness and creep play a major role and must be taken into account for prediction purposes. This work deals with a Discrete Element Method (DEM) to investigate mechanisms leading to interface delamination and fracture in TBC. Originally developed to model granular materials, DEM has been adapted to simulate continuous media using cohesive spring or beam elements. Thus, it has turned into a promising approach to simulate complex fracture phenomena arising in homogeneous or heterogeneous materials under mechanical or thermo-mechanical conditions [3,4]. In the present contribution, we take benefit of MULTICOR2D++ software developed at LTI laboratory to study a ceramic-metal multi-layer constituted of a plasma-sprayed ceramic TC and a NiCrAlY BC. Emphasis is first placed on thermo-mechanical stresses arising in TBC due to the mismatch of coefficients of thermal expansion. Effects of roughness are discussed using a unit cell in which the TC/BC interface has a sinusoidal profile. In a second step, interface delamination is investigated using a discrete Cohesive Zone Model (CZM) under mixed-mode conditions and failure is also examined in TC considering the Removed Discrete Element Failure (RDEF) process. Finally, similar simulations are performed on a realistic sample using a microstructure built by image processing. Such a model takes into account defects as pre-existent pores and cracks and an irregular TC/BC interface.

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