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# Discrete Element Method to predict cracks initiation and propagation in plasma-sprayed Thermal Barrier Coatings during a thermal cycle

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## Abstract

Thermal barrier coatings (TBCs) are advanced materials used in many industrial fields (aircraft engines, gas turbines, marine propulsion, etc.) to protect metal components from high operating temperatures. TBCs are multilayer materials consisting of a ceramic Top-Coat (TC) thermal barrier layer, a metal Bond-Coat (BC) intermediate layer between a superalloy substrate and the TC, and an oxidation-resistant layer called Thermally Grown Oxide (TGO). Predicting interface delamination and failure of the TBC under thermomechanical loading is quite complex due to the severity of the thermal conditions and the complexity of their microstructure, which includes microcracks, pores and heterogeneities. In addition, the lifetime of these systems is affected by several factors, including thermal expansion mismatch, oxidation, interface roughness and creep, which play a major role in the premature failure of TBC. In the present work, we consider a plasma-sprayed TC ceramic deposited on a NiCrAlY BC. Our main objective is to numerically simulate and reproduce the fracture mechanisms occurring during a three-stage thermal cycle comprising a heating phase from 25°C to 1100°C, a rest phase at 1100°C and a cooling phase from 1100°C to 25°C. For the numerical method, due to the heterogeneity of the TC ceramic layer and the complex cracks typically observed in TBCs, we opted for the discrete element method (DEM) which is a promising approach to simulate the mechanical and multiphysical properties of heterogeneous materials and predict their failure modes, including the propagation of complex cracks with coalescence and branching effects. First, an original visco-plastic creep model based on Norton's law is proposed. Then, the thermomechanical stresses induced by the combined effects of creep and thermal expansion coefficient mismatch are evaluated and compared with finite element method (FEM) calculations in the reference case of a TBC model with a sinusoidal profile. The effects of TGO thickness and amplitude are also investigated. Thirdly, the same study is applied to a realistic TBC model obtained by image processing and including defects such as pores, microcracks and an irregular TBC interface. Finally, the initiation and propagation of cracks occurring during thermal cycling are simulated in this context and the results are discussed in relation to experimental observations of the literature.

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