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Oxidation of high-temperature alloys. Application to failure of thermal barrier coatings

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ABSTRACT

Oxidation of high-temperature alloys represents complex, strongly-coupled, nonlinear phenomena which include: (i) diffusion of oxygen in the alloy; (ii) an oxidation reaction in which the reaction product causes substantial permanent, anisotropic volumetric swelling; (iii) high-temperature elastic–viscoplastic deformation of the base alloy and the oxide; and (iv) transient heat conduction. We have formulated a continuum-level chemo-thermo-mechanically coupled theory which integrates these various nonlinear phenomena. We have numerically implemented our coupled theory in a finite-element program, and we have also calibrated the material parameters in our theory for an Fe-22Cr-4.8Al-0.3Y heat-resistant alloy experimentally studied by Tolpygo et al. (1998). Using our theory we simulate the high-temperature oxidation of thin sheets of FeCrAlY and show that our theory is capable of reproducing the oxide thickness evolution with time at different temperatures, the permanent extensional changes in dimensions of the base material being oxidized, as well as the development of large compressive residual stresses in the protective surface oxide which forms. As an application of our numerical simulation capability, we also consider the oxidation of an FeCrAlY sheet with an initial groove-like surface undulation, a geometry which has been experimentally studied by Davis and Evans (2006). Our numerical simulations reproduce (with reasonable accuracy) the shape-distortion of the groove upon oxidation, measured by these authors. The ramifications for delamination failure of a ceramic topcoat on a thermally grown-oxide layer in thermal barrier coatings are discussed.