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Macro and Micro Residual Stresses in Zirconium Oxide Layers

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Introduction

Residual stresses are generally derived from experimental strain measurements through analytical calculations. These calculations rely on assumptions upon the mechanical characteristics of the oxide layers, in particular their isotropy. However, their microstructures are usually characterised by morphological and crystallograhic textures. The aim of this work is to study the influence of some microstrutural parameters on the evaluation of the residual stresses in zirconium oxide layers by finite element computations.

Guidelines

The influence of the oxide layer microstructure has been studied at two scales. At the oxide/substrate system scale, the oxide layer is viewed as a homogenous media but with thermo-elastic properties derived from its polycrystalline microstructure. Each grain of the polycrystal is assumed to be monoclinic zirconia since this is the crystal phase mostly developed during the zirconium oxidation. Two crystallographic distributions are considered for the polycrystalline aggregate: the isotropic distribution and one ideal fiber texture [1]. The thermo-elastic properties of these two microstructures were obtained thanks to the Voigt and Reuss bounds. Finally, these properties were used into finite element analyses of the stresses developed in the oxide-layer / substrate system during thermal loadings.

At the microstructural scale, we studied the influence of the morphological and crystallographic textures of the oxide layers by performing finite element analyses of Representative Volume Elements of their microstructures. RVE with equiaxed or columnar grains [2] were modeled by Voronoï polyhedrons (see Figure 1), each grain behaving as monoclinic zirconia [3][4]. The effective thermo-elastic properties of these RVE were computed and compared to the estimates given by the homogenization model. Moreover, intragranular stress distributions were also studied, showing that the stress level may be locally much higher than its mean value in the layer.

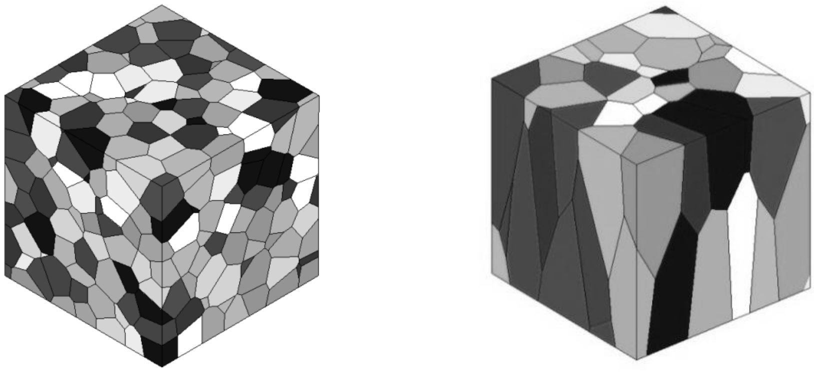

Figure 1: RVE of polycrystalline aggregates (512 equiaxed and 74 columnar grains)

Conclusions

First, the comparisons between the computations achieved at the layer/substrate system scale and the results given by the analytical formulas commonly used to derive the residual stresses from strain measurements are in good agreement as long as the assumptions on the thermo-elastic properties of the oxide layer remain valid. If not, the residual stress evaluated with these formulas may be very different from what have been computed.

Second, computations on RVE gave estimates of the effective properties of the polycrystalline aggregates of zirconia in good agreement with those given by the homogenization model. These computations also confirmed the influence of the crystallographic texture on the mechanical behavior of the oxide layer, but showed no influence of the morphological one. Last, the analysis of the intragranular stress distribution showed that the maximal stress may be 30% higher than its mean value in the layer. This stress level should be integrated to the failure analysis of the zirconium oxide layers.

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