Micromechanical Modeling and Simulations of the Effects of Oxygen in Titanium Alloys

Patricia Vernier*†[1], Aldo Marano[1], Lucille Bornowsky[1], and Pascale Kanoute[1]

[1]ONERA – DMAS, ONERA, Université Paris Saclay F-92322 Châtillon - France – France

Abstract

Titanium alloys are widely employed for aerospace applications due to their good thermomechanical performances and their lightweight. However, because of their capacity to dissolve oxygen, Titanium alloys may not withstand environments as extreme as temperatures exceeding 600∘C. During the oxidation of the material, oxygen diffuses from the free surface into the depths, where its presence significantly alters the mechanical properties. Particularly, the fatigue life is considerably reduced due to the initiation of cracks at the surface, where the highest oxygen concentrations are found. Therefore, it is crucial to understand the effects of oxygen over the microstructure for accurate predictions of the mechanical behavior of Titanium. Precisely, crystal plasticity models are used to describe the microstructural mechanisms implied in the deformations of such materials. In this work, we propose a methodology to account for the presence of oxygen in crystal plasticity FFT simulations of Ti6242 polycristalline aggregates under cyclic loadings. Our results are then compared to experimental data.

The insertion of oxygen in Titanium results in the increase of elastic anisotropy (3) (4), but also the increase of critic resolved shear moduli (CRSS) (1) (2). Since the oxygen concentration varies in the material with respect to the surface, it is essential to characterize this dependence at the microstructural scale. We thus rely on available nanoindentation experiments data that give indirect estimates of these parameters through the measurement of reduced elastic and hardness moduli. Hence, we can identify and quantify the dependence of the elastic moduli to oxygen concentration by following (4). The identification procedure of these authors is based on a model developed in (5), which provides a relationship between the reduced elastic modulus and the elastic moduli through the displacement of the indent. Similarly, we consider that the CRSS values are related to the measures of hardness. The variation of the material parameters with respect to the oxygen content can then be implemented in the setup of numerical simulations.

Finally, we perform crystal plasticity full-field simulations of Titanium alloys using the massively parallel FFT-based solver AMITEX_FFTP, on both reference and oxidized material. The morphology and texture of the Representative Volume Element are generated from EBSD analyses. We first identify the global behavior of our model by comparison with experimental tensile tests. Next, we focus on the effects of free surfaces under cyclic loadings, which is essential for understanding the deformation mechanisms that lead to crack initiations. The analysis of local fields obtained numerically, in conjunction with experimental

*Speaker

†Corresponding author: patricia.vernier@onera.fr

observations of surface fractures, provide a deeper insight into the microstructural mechanisms underlying reduction of fatigue life.

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