A Combined Micromechanical and Crystal Plasticity Approach to Predict Oxygen Embrittlement in Ti-6Al-2Sn-4Zr-2Mo

Aldo Marano[1], Lucille Bornowsky[1], Patricia Vernier[1], Aurélien Vattré[1], Abdelali Oudriss[2], Xavier Feaugas[2]

[1] DMAS, ONERA, Université Paris Saclay, F-92322 Châtillon, France
[2] Laboratoire des Sciences de l'Ingénieur pour l'Environnement, La Rochelle University, UMR-CNRS 7356, Avenue Michel Crépeau, 17042 La Rochelle, France

aldo.marano@onera.fr[1]

INTRODUCTION

Titanium alloys operating at elevated temperatures are susceptible to oxygen ingress during oxidation, leading to the formation of an oxygen-enriched subsurface zone characterized by severe embrittlement [1]. This oxygen-affected zone (OAZ) exhibits dramatically altered mechanical properties and represents a critical damage precursor in structural components. Understanding the mechanisms governing crack initiation in the OAZ is essential for reliable lifetime prediction of titanium alloy components. This work presents a comprehensive methodology combining advanced micromechanical characterization with crystal plasticity modeling to predict crack formation stress levels in tension in the OAZ of the Ti-6Al-2Sn-4Zr-2Mo (Ti6242s) alloy.

MICROMECHANICAL CHARACTERIZATION

The experimental characterization strategy employs micromechanical testing on oxidized Ti6242s samples. Prior to testing, the oxide layer was removed by polishing to enable direct observation of deformation and damage mechanisms within the OAZ itself. In-situ SEM micro-tensile experiments revealed a lack of plastic deformation within the OAZ, accompanied by crack formation. They critically enabled measurement of the stress at which these cracks form (Figure 1 a). To quantify the mechanical property gradient induced by oxygen diffusion, nanoindentation measurements were performed on cross-sections of oxidized specimens. These measurements revealed that both hardness and stiffness strongly increase with oxygen intake across the OAZ (Figure 1 b), with the hardness increase being more pronounced than the stiffness increase. The systematic mapping of mechanical properties provided essential input data for subsequent numerical modeling.

MODELING

The modeling framework employs crystal plasticity simulations to capture the complex mechanical response of the heterogeneous oxygen-affected microstructure. A crystal plasticity constitutive model was calibrated against experimental tensile curves of the reference Ti6242s alloy. Subsequently, large-scale crystal plasticity simulations were performed, based on a representative polycrystalline microstructure with a free surface. The effect of oxygen was accounted for in the simulation by modeling the property gradient within the OAZ. In this way, the stiffness matrix and critical resolved shear stresses of the crystal plasticity laws have been calibrated to reproduce the increase in hardness and stiffness measured with nanoindentation mapping.

The simulations revealed substantial stress gradients developing within the OAZ under the applied tensile loading, reflecting the mechanical property mismatch between the embrittled surface layer and the underlying alloy (Figure 1 c). Using a cleavage-based failure criterion within the OAZ, the predicted critical stress for crack initiation in tension showed good agreement with the crack formation stress measured experimentally from the micro-tensile tests. This demonstrates that the combination of experimentally measured property gradients with crystal plasticity simulation successfully captures the micromechanical conditions governing crack initiation in the OAZ.

CONCLUSIONS

This integrated experimental-numerical framework represents a first step towards accurate microstructure-informed prediction of oxygen embrittlement in titanium alloys. Perspectives for extending this methodology to more complex loadings will also be discussed.

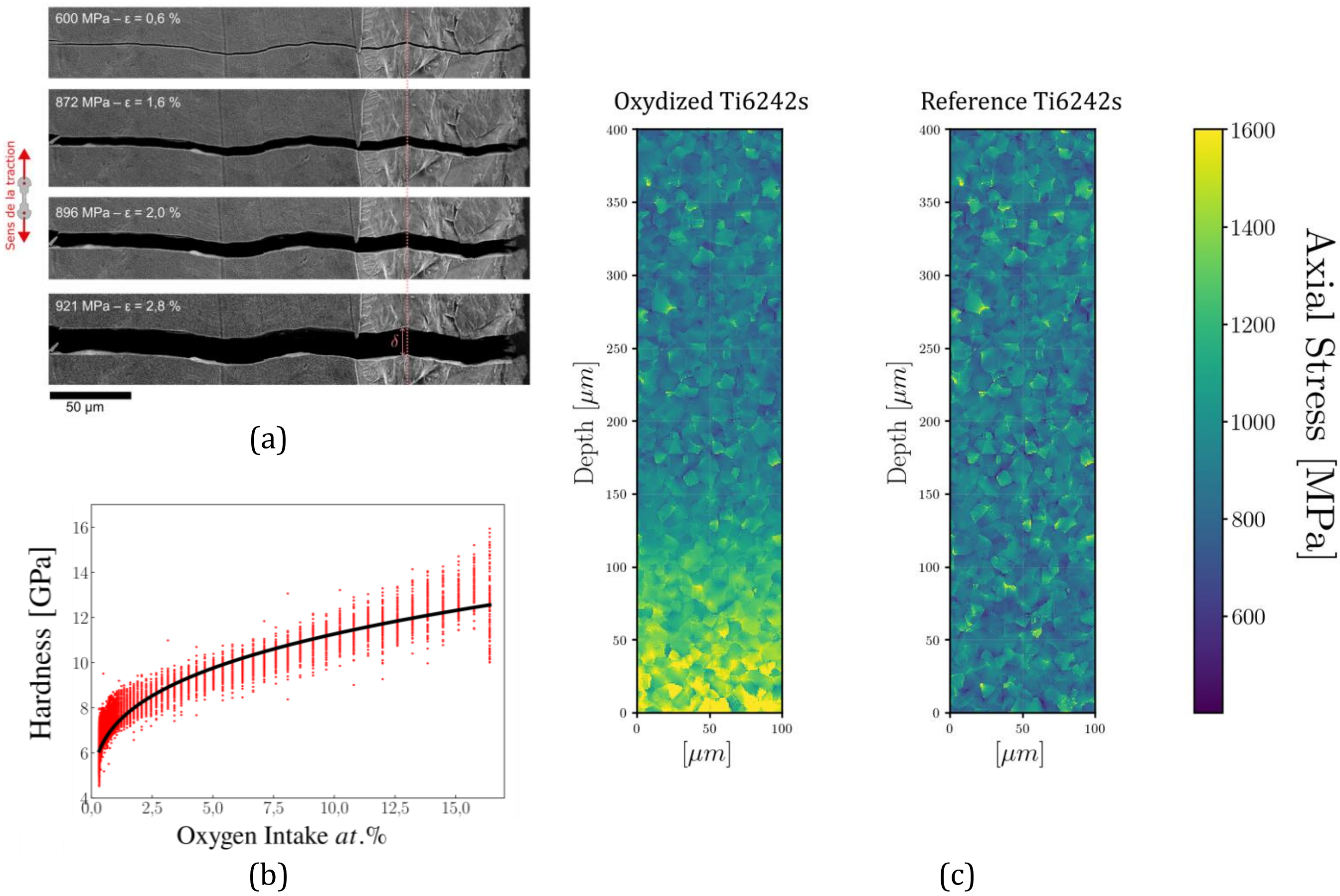

Figure 1 : In-situ observation of crack formation and opening in the OAZ during microtensile testing (a) Hardness evolution with oxygen intake characterized via nanoindentation mapping (b) stress fields obtained via crystal plasticity simulations informed with the OAZ property gradient (c)

[1] Pilchak, A. L., W. J. Porter, and R. John. "Room temperature fracture processes of a near-α titanium alloy following elevated temperature exposure." *Journal of Materials Science* 47.20 (2012): 7235-7253.