Coupled diffusion-mechanics modeling of titanium alloys under high temperature oxidizing conditions

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Abstract

High temperature oxidation of titanium alloys induces substantial oxygen diffusion beneath the oxide scale, forming an oxygen-affected layer (OAL). The stiffness and hardness of alpha-titanium strongly increase with increasing oxygen concentration. The increase in stiffness is known to be strongly dependent on crystal orientation (1), as well as the swelling deformation induced by oxygen intake (2). Compared to the bulk, the OAL is thus characterized by a strong alteration of mechanical properties, that is strongly microstructure dependent. Pre-oxidation has been shown to significantly influence the alloy mechanical response, that evolves towards an embrittlement associated with the evolution of deformation and damage mechanisms at the microstructure scale, particularly in the OAL. Finally, recent results show that oxygen diffusion in the alloy may be affected by a mechanical stress imposed during oxidation (3). Due to these strong interactions, it is necessary to account for the influence of oxygen diffusion when analyzing mechanical tests conducted with in-situ oxidation of the alloy. These encompass, for instance, creep and low-frequency fatigue tests at high temperatures.
To gain new insights into these phenomena, this study presents a novel model coupling diffusion and mechanics to simulate the behavior of quasi-alpha titanium alloys. The model accounts for the effects of pressure and of the pressure gradient on oxygen transport. An eigenstrain is included to account for swelling deformation effects caused by oxygen intake. The material's mechanical behavior is described using a crystal plasticity framework. The elastic and plastic properties evolve as a function of the local oxygen concentration, in order to describe stiffening, hardening, and the evolution of elastic and plastic anisotropy in the OAL. This comprehensive coupling of diffusion and mechanics provides a robust foundation for understanding the complex interactions between oxygen ingress, microstructure, and deformation mechanisms. The model is solved by coupling a finite-difference scheme for the diffusion-transport equation, to a non-linear FFT-based mechanical solver. It has been implemented within the massively parallel spectral solver AMITEX_FFTP to enable the simulation of large and complex microstructures with high computational efficiency.

This framework is applied to study the behavior of the Ti6242s alloy in an oxidizing environment at 600∘C. The simulation of creep tests with in-situ oxidation preceded or not by a pre-oxidation phase is studied. In particular, the influence of the various model features and parameters on mechanical properties and deformation heterogeneities is examined. Finally, in the light of comparison with recent experimental findings, their suitability is discussed to pave the way for an improved understanding of the material's mechanical response during oxidation.

*Speaker

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