The 8th European Congress on Computational Methods in Applied Sciences and Engineering
ECCOMAS Congress 2022
5 – 9 June 2022, Oslo, Norway

A multi-physics finite element framework for diffusion-assisted intergranular fracture of polycrystals

Kim Louisa Auth[1], Jim Brouzoulis[1] and Magnus Ekh[1]

[1] Chalmers University of Technology, Hörsalsvägen 7 41296 Göteborg, Sweden
kim.auth@chalmers.se, jim.brouzoulis@chalmers.se, magnus.ekh@chalmers.se
www.chalmers.se

Key Words: *Multiphysics, Polycrystals, Stress-assisted oxidation, Oxygen embrittlement*

Critical gas turbine components, often fabricated from nickel-based superalloys, need to withstand significant loading, high temperatures as well as an oxygen-rich environment. Predictions of the material behavior are crucial in the design process of such components.
Polycrystalline nickel-based superalloys experience a shift from transgranular ductile fracture to intergranular brittle fracture when exposed to a combination of high temperatures, oxygen-rich environment, and tensile mechanical loading (see e.g. [1]). This phenomenon can be explained by the multi-physics interaction of oxygen diffusion into the grain boundary ahead of the crack tip and mechanical deterioration of the grain boundary by the presence of oxygen.

We propose a thermodynamically consistent fully chemo-mechanically coupled modelling framework for intergranular fracture. A coupled cohesive finite element formulation is employed for modelling the grain boundaries. The model captures the full coupling between mechanical degradation of the grain boundaries by oxygen and mechanically enhanced diffusion of oxygen ahead of the crack-tip. For the latter, the model of stress-assisted diffusion [2] is adapted to cohesive zone modelling, leading to enhancement of the oxygen diffusion by the gradient of normal traction rather than the gradient of hydrostatic stress. Further, the modelling framework allows for mixed-mode loading / unloading scenarios. A crystal plasticity model is adopted for the grains.

Numerical experiments are performed on 2D polycrystalline structures. Convergence behavior of the monolithic solver, as well as required mesh and time step sizes are discussed. Finally, we show that the model can qualitatively predict experimental results such as: reduction of ultimate tensile strength, accelerated crack growth due to dwell time combined with mechanical loading and saturation of crack growth rates for increasing environmental oxygen pressure levels.

REFERENCES

[1] Pfaendtner, J. A., & McMahon, J. J. (2001). Oxygen-induced intergranular cracking of a Ni-base alloy at elevated temperatures - An example of dynamic embrittlement. *Acta Materialia*, *49* (16), 3369–3377. https://doi.org/10.1016/S1359-6454(01)00005-2

[2] Sofronis, P., & McMeeking, R. M. (1989). Numerical analysis of hydrogen transport near a blunting crack tip. *Journal of the Mechanics and Physics of Solids*, *37*(3), 317–350. https://doi.org/10.1016/0022-5096(89)90002-1