Phase Field Modelling of Ni oxidation and YSZ cracking in Solid Oxide Cells

Sylvain Fournier*[1], Maxime Hubert[1], Gergely Molnár[2], Aurélien Doitrand[3], Sylvain Meille[3], and Jérôme Laurencin[1]

[1]CEA Liten – CEA Liten – France

[2]Laboratoire de Mécanique des Contacts et des Structures [Villeurbanne] – Institut National des Sciences Appliquées (INSA) - Lyon – France

[3]Matériaux, ingénierie et sciences [Villeurbanne] – Université de Lyon, INSA de Lyon, Laboratoire MATEIS CNRS UMR 5510 – France

Abstract

Solid Oxide Cells (SOCs) are promising high temperature (700◦C-850◦C) energy conversion devices that present a high efficiency in both fuel cell and electrolysis modes and can be used in a wide range of technological applications. However, their widespread development is currently hindered by durability and reliability problems including various mechanical damage in the cell components such as electrodes and electrolyte (1).
The conventional 'hydrogen' electrode is a cermet of Nickel and Yttria Stabilized Zirconia (Ni-YSZ combining Ni electronic conductivity with YSZ ionic conductivity. Failure in the system (such as air reintroduction during the system shutdown, gas leakage or fuel overutilization due to a problem of gas feeding) leads to the Ni re-oxidation. The transformation from Ni to NiO results causes volumetric expansion within the pores and induces mechanical strain on the YSZ backbone, compromising its structural integrity and electrode functionality. Therefore, the robustness of the cell components still needs to be improved, especially for the cermet. However, the threshold in terms of Ni re-oxidation triggering the fracture in the cermet is not precisely known.

To better understand the involved mechanisms, a modelling approach is proposed to calculate the nucleation and the propagation of the micro-cracks in YSZ during Ni re-oxidation. We developed a phase field model (PFM) to simulate the Ni oxidation and the development of cracks in the YSZ backbone.

Regarding the Ni oxidation, the model takes into account the evolution of the Ni, NiO and porosity phases over time. Particular attention was given to integrate the specificities of the Ni oxidation mechanism, like the stress induced in the NiO layer as previously explored by Lin *et al.* (2). Unlike the majority of PFM oxidation models, our approach simultaneously tracks the evolution of two interfaces (Ni-NiO and NiO-porosity), following the framework established by Zaeem *et al.* (3), but applied to a complex 2D microstructure.

A previously developed (4) phase field model for YSZ backbone fracture is applied to microstructures at different oxidation times to evaluate the probability of their local cracking. For the model calibration and its validation, we compared the simulations with microscopy

*Speaker

images of cermet subjected to varying Ni/NiO oxidation states. The results showed that the oxidation model i) reasonably captures the expansion and kinetics of oxidation, despite over-simplifying certain characteristics of the NiO film and ii) satisfactorily reproduces localized cracking of the structure during oxidation.

This study demonstrates the potential of phase-field modelling to provide insights into SOC degradation mechanisms, paving the way for improved microstructure designs or identification of materials that allows mitigating the degradation.

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