Investigating Humidity Degradation in an SOFC Cathode through Multi-Scale Modeling

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Humidity in the air stream of the solid oxide fuel cell (SOFC) cathode has been shown to cause degradation in the electrochemical performance of the SOFC. Humidity in the cathode causes a two-stage degradation: an initial rapid decrease in the output voltage followed by a steady long-term voltage degradation over the operating lifetime of the cell. Experimental research has shown that water vapor reacts with the strontium-doped lanthanum manganite (LSM) cathode causing degradation in operating voltage [1]. Studies have also shown degradation in strontium-doped lanthanum iron cobalt oxide (LSCF) cathodes as well [2].

Studies of humidity in the cathode have considered the effects of humidity on the operation of the SOFC and the possible reaction mechanisms causing degradation. Two reaction mechanisms have been suggested between LSM and H_2O [1, 3]. One suggested reaction mechanism involves the reaction of lanthanum with water to form a lanthanum oxide nano-particle on the surface of the cathode [3,4]. Kim et al [3] found 100 nm particles on the surface of a mixed LSM/ScSZ cathode after five hours of electrochemical testing. Another possible reaction mechanism involves the reaction of manganese (Mn) with water [1,2]. Nielson et al [1] suggest a degradation of the cathode-electrolyte interface due to the reaction of Mn ions with water vapor; while Liu et al [2] suggest the formation of Mn oxide particles on the surface of the cathode.

To better understand the reactions of H_2O with LSM and their effect on the electrochemical performance of the SOFC we developed a multi-scale modeling approach which considers the micro-scale reactions on the LSM surface, the meso-scale reactive transport of H_2O in the cathode, and the macro-scale performance degradation in an SOFC stack. The micro-scale model uses molecular dynamics and density functional theory to investigate the reactions of LSM with H_2O. This work is focusing on the formation of Mn oxides. Based on the thermodynamics of the system the reaction of H_2O and Mn are the most likely form of the reactions between H_2O and LSM. The meso-scale model is investigating the reactive transport of H_2O in the porous cathode using the smoothed particle hydrodynamics (SPH) method which explicitly resolves the porous microstructure of the cathode. Finally, the macro-scale model is using the SOFC-MP [5] model to investigate the effects of humidity on long term stack performance.

The multi-scale modeling approach couples the micro-scale and meso-scale models via model parameters such as the activation energies of the reactions and diffusion coefficients in the cathode. The meso-scale model is then used to develop a continuum damage model which is implemented into the SOFC-MP stack model.

The models have been used to investigate several humidity degradation cases which correspond to accelerated testing conditions used in experimental studies [5]. The meso-scale model was used to simulate 100 hours of SOFC operation to develop a damage model based on the coverage of H_2O on the LSM surface, Figure 1. The functional damage model was then implemented in SOFC-MP to investigate the effects of humidity on long term electrochemical performance, Figure 2.

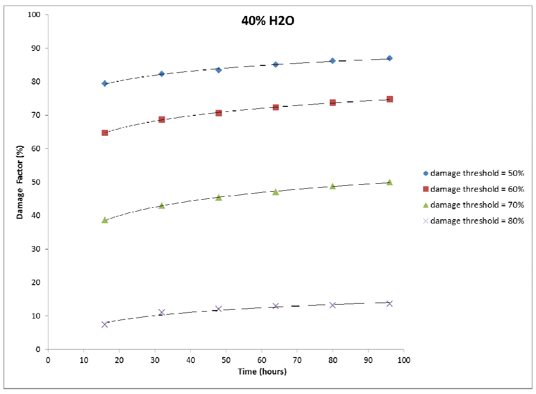

Figure 1: Damage factor over time as predicted by the meso-scale model.

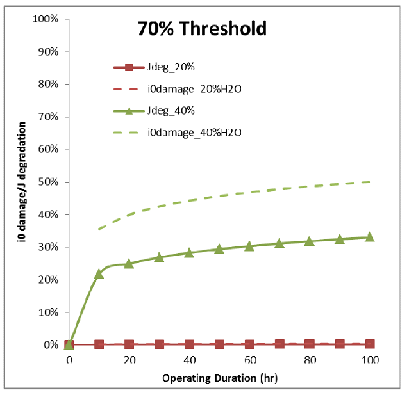

Figure 2: Stack level model of long term performance for 40% humidity.

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