Prediction of secondary-phase formation and degradation in solid oxide fuel cell anodes

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Insufficient lifetime is a major factor impeding the large-scale commercialization of solid oxide fuel cell (SOFC) technology. The formation of secondary phases in the porous electrodes can occur via various chemical mechanisms and represents a major cause of degradation due to pore clogging and deactivation of active surfaces. We present a modeling and simulation study of secondary-phase formation in porous Ni/YSZ-based anodes. Specifically, we investigate the formation of solid nickel oxide (reoxidation) in the case of high fuel utilization or low cell voltages, as well as the formation of solid carbon (coking) in the case of external and internal reforming.

The model is based on a multi-phase framework [1] that allows the introduction of arbitrary solid phases (here: Ni, YSZ, NiO, Carbon) plus the gas phase. Reactions between the bulk phases are modeled via interface-adsorbed species and they are described by an elementary kinetic approach. Published experimental data are used for parameterization and validation. The dynamic model is applied to predict and analyze nickel oxidation and carbon formation in one and two dimensions as function of operating condition and cell design. Simulations show that nickel oxidation can cause a hysteretic behavior in the current/voltage behavior. Carbon deposition occurring at open circuit under reformate fuel operation can lead to a continuous decrease in open-circuit voltage. Critical operating conditions are identified and discussed.

[1] J. P. Neidhardt, D. N. Fronczek, T. Jahnke, T. Danner, B. Horstmann, and W. G. Bessler, *J. Electrochem. Soc.* 159, A1528-A1542 (2012)