Topological Evolution of SOFC Electrode Materials: A Microstructural Perspective

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A solid oxide fuel cell (SOFC) anode is a complex three-phase microstructure within which all phases (pore, conducting metal and ceramic oxide) form contiguous networks. State-of-the-art SOFC anodes consist of yttria stabilized zirconia (YSZ) as the ceramic material and nickel (Ni) as the metallic phase. Recent experimental findings suggest that SOFC anodes undergo a series of morphological evolutions that tend to degrade cell performance. In particular, Ni phase coarsening, an interface driven phenomenon, under operating temperatures leads to a total reduction in the density of three phase boundary (TPB) lines. Furthermore, the re-distribution of Ni, electron-conducting phase, within the anode during coarsening can have a profound effect on the contiguity of Ni phase and the resulting electron transport paths in the anode.

In this study, we examine the effects of the local microstructure on the overall stability of SOFC anodes under extended use and operating temperatures. To this end, we present a continuum phase-field model capable of capturing the coarsening behavior of Ni in multi-phase SOFC anodes. The model also accounts for the polycrystalline nature of Ni along with the Ni interaction with the YSZ skeleton.

In order to identify morphological parameters that play a key role on the stability of Ni phase, a systematic study of the effects of the Ni phase characteristic length scales on the coarsening rate was conducted. Several topological attributes, such as Ni particle size distribution, three-phase boundary lines and contiguity degree were monitored as SOFC anode systems evolved over time. Simulation results provide future avenues that can be utilized to design the next generation of stable SOFC microstructures. This work is supported by the Energy Frontier Research Center on Science Based Nano-Structure Design and Synthesis of Heterogeneous Functional Materials for Energy Systems funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences (award DE-SC0001061).