

### **Multiscale Assessment of Charge and Mass Transfer in Solid Oxide Cells**

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**ABSTRACT** Solid oxide cells are solid state electrochemical energy conversion devices that can be operated as fuel cells or electrolyzers. Solid oxide fuel cells (SOFCs) provide direct conversion of chemical energy to electrical energy using diverse fuels. Under applied electric current solid oxide cells serve as solid oxide electrolyzers for fuel and oxygen generation. Solid oxide cells are composed of a dense electrolyte bounded by porous composite electrodes. The composite electrodes of solid oxide cells are inherently multiscale material systems composed of distinct solid and pore phases. These phases support the transport of ions, electrons, and gaseous reactants that feed electrochemical reduction and oxidation reactions. Within the microstructure discrete particles that comprise solid oxide electrodes form grains and grain boundaries that influence charge transport. Assemblies of sintered grains form conducting networks that span from submicron domains to electrode thicknesses on the scale of millimeters. Charge transport in the solid phase is coupled to transport of gaseous reactants through a network of open pores by electrochemical reactions. This arrangement creates a multiscale charge and mass transport interaction spanning from the grain boundary (nm) to device scale (mm). Computational and analytical methods for addressing this multiscale transport problem are addressed. A mesoscale model is presented for the rapid assessment of electrode performance. This mesoscale analysis is founded on analytical charge transport models that treat particles within the electrode as electrochemical fins, i.e. extended surfaces of ion conducting material subject to a surface charge transfer reaction. This method is applied to both phenomenological structures and 3D microstructural imaging data obtained using with x-ray nanotomography. Comparison with finite element models of charge transport within the microstructure demonstrates the accuracy and computational efficiency of the electrochemical fin approach. Analysis at microstructural scales is complemented by macroscopic solid oxide cell mass and charge transport models that demonstrate trade-offs inherent in design of microstructure, bulk electrode geometry, and current collector geometry. Predictions of charge and reactant distributions provide a route toward understanding performance and degradation driven by local reactant concentrations and electrochemical potentials. The combination of these techniques provides an approach for the rapid and effective assessment of solid oxide cell performance that accounts for the effects of multiscale geometry.