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An Analytical Performance Assessment Tool for Complex Reticulated 3-D Electrochemical Electrode Microstructures

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Electrochemical energy storage and conversion devices, including fuel cells and batteries, rely upon distinct 3-D arrangement of chemically active materials and phases in the electrode to support transport of reactants and charge. The ability for directed design of these materials at the micron and nanometer scale to create more effective reaction sites and supply reactant species to these sites holds the potential for enhanced device performance and longevity. Although various approaches, ranging from percolation theory and mixture average models, to detailed multiphysics models have been proposed [1], current approaches have considerable shortcomings, ranging from mixture average models that cannot accurately correlate predictions with a specific microstructure, to detailed multiphysics models that make analysis intractable for computational domains large enough to be representative of the actual material. There is a scientific gap and need for a computationally tractable tool that can accurately predict the performance of complex 3-D reticulate material structures used in electrochemical devices.

In this presentation, an analytical model capable of rapidly and accurately assessing the performance of complex 3-D microstructures will be reported [2]. This rapid assessment tool, called Electrochemical Fin (ECF) theory, can account for the 3-D shape of the microstructure, surface electrochemical reactions, and ion/electron diffusion in the bulk material. This approach, as illustrated in Figure 1, uses analytical closed form solutions to accurately represent the material microstructure as a detailed 3-D network. The actual 3-D material microstructure is imaged and characterized using a synchrotron-based transmission x-ray microscope. Three-dimensional structures within the sample volume are imaged and tomographically reconstructed at sub-20 nm spatial resolution.

ECF theory is demonstrated on $Sr_2Fe_{1.5}Mo_{0.5}O_{6-\delta}$ (SFM), a redox stable solid oxide fuel cell (SOFC) electrode [3]. X-ray nanotomography performed is using a synchrotron-based transmission x-ray microscope with subsequent image processing to obtain 3-D data networks of resistive components and determining appropriate model parameters is presented. The electrode microstructural network is then subsequently analyzed using ECF theory. Predictions of electrode performance compare favorably to 3-D finite element simulations of charge transport with surface electrochemical reactions. Analysis of larger representative volume elements extracted from the x-ray nanotomography data agrees reasonably with experimental measurements of polarization measurements [2]. Advantages of ECF theory will be addressed, particularly with respect to the significant reduction in memory requirements

and computational time. ECF is able to rapidly analyze real microstructures with details comparable to finite element and lattice Boltzmann methods, but at volume sizes that finite element and lattice Boltzmann methods cannot perform due to memory and computational time limitations.

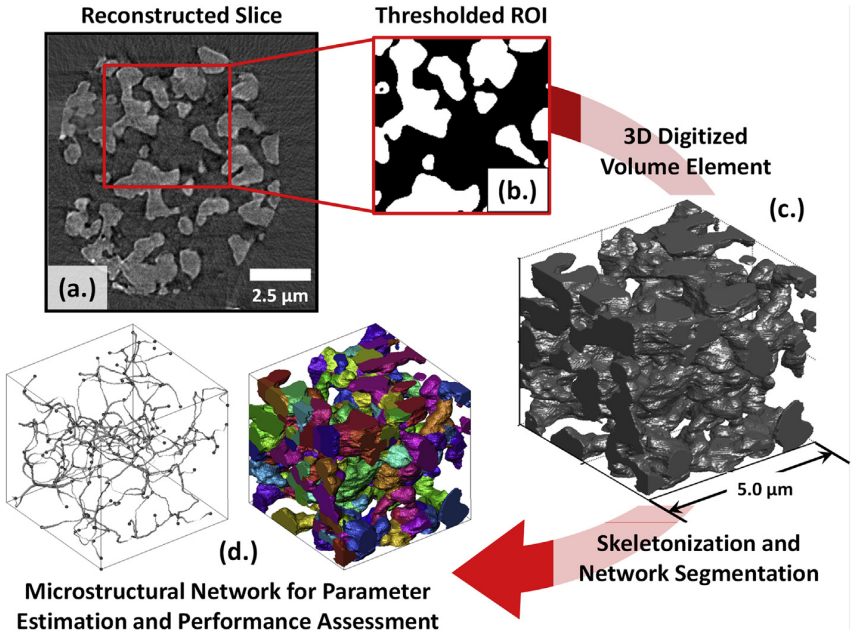

Figure 1: General process workflow for generating an electrochemical fin network from a real $Sr_2Fe_{1.5}Mo_{0.5}O_{6-d}$ (SFM) electrode microstructure: (a) X-ray nanotomography data is reconstructed to generate a grayscale tomogram; (b) a region of interest within the grayscale image data is thresholded to produce a digitized volume element representing the distinct phases of the electrode; (c) the digitized data is passed to a skeletonization algorithm and an initial microstructural skeleton is further partitioned into a network; (d) the particles comprising the network are characterized to yield electrochemical fin morphological parameters and the network performance is subsequently assessed. Figure is from [2].

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