Quantifying the Nature and Impact of Mesoscale Heterogeneities in SOFC Electrodes

Motivation
• Key factors limiting the commercialization of SOFCs:
  1. High cost of manufacture
  2. Poor reliability
  3. Low durability
• A tradeoff exists between cost of manufacture and reliability / durability of electrodes.

Quantitative Analysis of Heterogeneities in Electrode Microstructures

Pillars for PFIB-SEM

Experimental Microstructures

Synthetic Microstructures

Semi-empirical Model for Quantitatively Rationalizing Origin of Heterogeneities

Model Fit to Experimental Datasets

Locally-resolved Simulations of Microstructures

Microstructure-based Simulations
• Effective medium theories only output averaged performance values and assume relatively high homogeneity within a volume
• Degradation is strongly dependent on local electrochemistry, which can be studied with microstructure-based, locally resolved simulations
• Commercial fuel cell exhibits various types of microheterogeneities that do not conform to effective medium theory assumptions
• Microstructure-based simulations of heterogeneous electrodes require advances in:
  ❖ large-volume, high-resolution 3D reconstructions
  ❖ morphology preserving meshes that capture 2 and 3 phase boundaries and that can be automated
  ❖ massively-parallel, multi-physics, finite-element codes implemented on high performance computers

Conclusions
• Reconstructions of commercial grade SOFC electrode microstructures using PFIB-SEM confirmed heterogeneity exists over multiple length in theses electrodes.
• Combining experimental microstructures with a large number of synthetic ones a semi-empirical model is presented that quantifies microstructural variations present in the electrode microstructures.
• A high-throughput microstructure base finite element approach is developed to study the impact of heterogeneities on the statistical variation in local property.
• The model confirms that the heterogeneous commercial electrodes exhibit more performance hotspots than the less heterogeneous synthetic ones.