Microscopy Supported Multi-Scale Modeling of PEM Fuel Cells

Abstract for the 231st ECS meeting in New Orleans (May 2017)

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Proton exchange membrane fuel cells (PEMFCs) are being developed as alternative energy sources for both residential and automotive applications. For this technology to reach its full commercial potential, however, a significant reduction in cost is still required while the performance and durability of PEMFCs being maintained or improved. The key in this process is continuous improvement of membrane electrode assembly (MEA) through both the development of new materials and the optimization of the 3D structural arrangement of individual MEA components [3,4,5,7]. Structural optimization of MEA remains to be challenging due to multiple materials interacting across 6 orders of magnitude in their characteristic length scales, from several nanometers for the catalyst particle size to hundreds of micrometers for carbon fibers in porous transport layer.

In recent years, several microscopy techniques have become widely available to characterize the three-dimensional (3D) structure of PEMFC catalyst layers. Due to the heterogeneous nature of the PEMFCs sample, a correlative, multi-scale imaging protocol is developed in this work. The following technology is used where their corresponding resolution limit is pushed.

- Transmission Electron Microscope tomography, TEMt [2] (0.60nm X 0.60nm X 0.60nm Voxel Size)

- Focussed Ion Beam - Scanning Electron Microscope tomography, FIB-SEM [6] (2.5nm X 2.5nm X20 nm Voxel Size)
- Micro and Nano X-ray Computed Tomography, NanoCT [1] (367nm X 367nm X 367nm Voxel Size)

Each technique by itself supports valuable insight to be obtained on the investigated structure at the corresponding length scale. By combining 3D imaging data at multiple scales, an unified structural characterization workflow is developed. Furthermore, an up scaling approach are developed based on TEMt, SEM and NanoCT reconstruction of catalyst layer, micro-porous layer and porous gas transport layer of a PMEFC cathode. Structural properties and effective transport properties are computed at each scale via image-based numerical simulation. Effective transport properties are up-scaled. MEA performances are predicted based on the obtained effective quantities at micro-scale.

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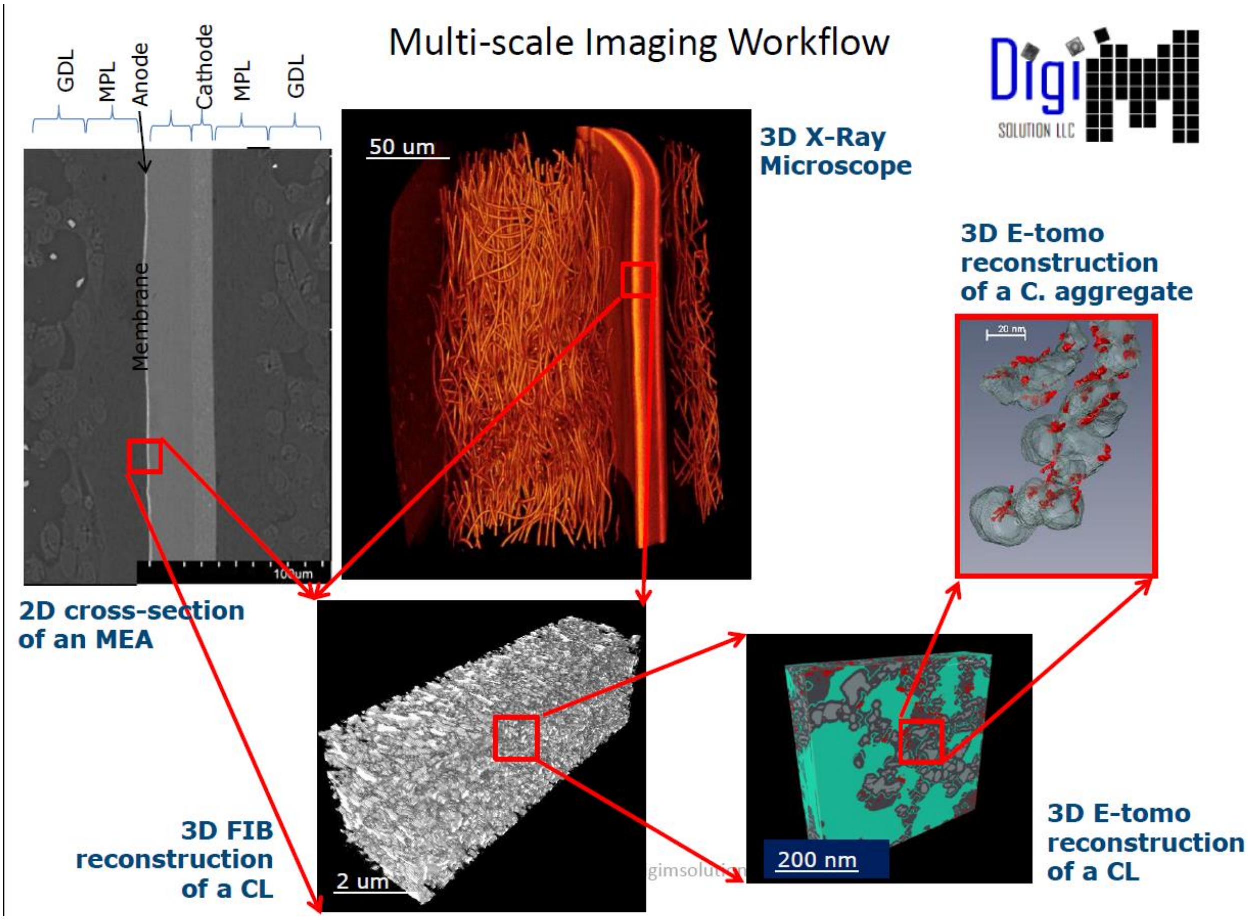

Multi-scale Imaging Workflow
GDL
MPL
Anode
Cathode
MPL
GDL
Membrane
100um
50 um
3D X-Ray Microscope
3D E-tomo reconstruction of a C. aggregate
20 nm
2D cross-section of an MEA
3D FIB reconstruction of a CL
2 um
200 nm
3D E-tomo reconstruction of a CL