Ionomer Reconstruction in Three-dimensional Digital Images of Catalyst Layer Microstructure of PEM Fuel Cells

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Résumé

1 Introduction

Proton exchange membrane fuel cells (PEMFCs) have emerged as a promising alternative energy source, offering clean and efficient power generation for various applications. A crucial component of PEMFCs is the catalyst layers (CL), where electrochemical reactions take place, converting hydrogen and oxygen into water and electricity. Within the CL, the complex interplay of catalyst, ionomer, and carbon support, governs the overall performance and durability of the fuel cell.

Among these components, the ionomer plays a pivotal role by enabling the transport of protons while simultaneously ensuring the necessary mechanical stability and water management within the CL. Understanding the spatial distribution and behaviour of the ionomer within the CL is of utmost importance for optimizing the fuel cell performance and improving its design.

In this work, we present a numerical approach to reconstruct the ionomer distribution in three dimensional images of the CL microstructure obtained by FIB-SEM imaging.

2 Methodology

The CCL used in this study is a TEC10E50E with high surface area (HSA) carbon from Tanaka. To analyse its structure, 3D FIB-SEM data was collected using a Zeiss Crossbeam 550 microscope. The imaged volume had dimensions of 13.2 μm by 10.95 μm by 5.24 μm, with a spacing of 5 nm between slices and a pixel size of 5 nm, resulting in cubic voxels measuring 5 nm^3. The process of segmenting the three-dimensional image into solid voxels and void voxels uses a combination of techniques described in references (1) and (2).

However, the current segmentation procedure does not allow for the separation of the ionomer (I) from the carbon black and platinum (Pt/C). Consequently, a numerical approach that incorporates several algorithms is developed to identify the distribution of the ionomer within

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the image consistently with high resolution TEM images ((3), (4)). In particular, a local size filtering of the solid phase inclusions, and a coverage model based on the computation of the 3D local curvature of the solid phase are developed to identify the ionomer in two forms: filament ionomer that partially occupies the pore space, and ionomer thin films that coat the platinum-loaded carbon phase.

3 Results

An illustrative example of the computed ionomer distribution is shown in figure.1. The reconstruction leads to an ionomer distribution forming a well-connected percolating network across the thickness of the cathode catalyst layer. The obtained reconstructed images are currently used to compute effective transport properties of the considered CL.

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