Simulation of carbon black aggregate and evaluation of ionomer structure on carbon in catalyst layer of polymer electrolyte fuel cell

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HIGHLIGHTS

- Actual carbon black structure is simulated and the validity of this is confirmed.
- Ionomer distribution on carbon black and in catalyst layer is estimated.
- Correlation equation of ionomer thickness, coverage and conductivity are obtained.

ARTICLE INFO

ABSTRACT

In polymer electrolyte fuel cells (PEFCs), an ionomer is needed to maintain the proton conductivity in the catalyst layer; however, it causes oxygen diffusion resistance because of its thickness on the platinum surface and the blockage of the void spaces. Therefore, understanding the ionomer distribution on a platinum/carbon black (CB) support catalyst is extremely important, because this knowledge can contribute to a reduction in the resistance for the cathode oxygen reduction reaction. In this study, a three-dimensional CB aggregate structure is simulated using numerical analysis with various experimental information (surface volume, aggregate size, and anisotropy); from the viewpoint of the roughness and morphology of CB, the ionomer distribution on its surface is simulated. The relationship between the ionomer content and the coverage of the ionomer on carbon is determined. Moreover, the effect of the surface structural properties on the ionomer distribution in the catalyst layer is studied using simulations. Based on the results, the relationship between the surface roughness and the ionomer connectivity is determined. The coverage and thickness of the ionomer do not change linearly upon changing its content. This condition strongly depends on the surface roughness. Insights gathered from this study can assist in designing optimum catalyst layer.

1. Introduction

Polymer electrolyte fuel cells (PEFCs) are candidate power sources for future automobiles that will utilize hydrogen energy, known as Fuel Cell Vehicles (FCVs). The most important advantage of PEFCs is the low operating temperature. Therefore, they are more suitable for automobiles than a stationary power supply. The most important issue in popularizing FCVs is reducing the cost of a PEFC stack. The major part of the cost of PEFCs is associated with the platinum particles on the electrode catalyst. To reduce the cost of PEFCs and achieve the target cost, it is necessary to develop new materials such as low- and non-platinum catalysts, and improve the platinum utilization [1]. If proton and oxygen don't transfer on the surface of Pt catalyst, this Pt catalyst is not used for reaction. And the Pt utilization, which is the unused Pt surface ratio per all of Pt surface area in catalyst layer, decreased. An improvement in the platinum utilization will reduce the stack cost because the quantity of supported platinum will decrease. In current PEFCs, the reaction and transport resistance in the oxygen reduction reaction (ORR) at the cathode are the rate-limiting factors, thus, the development of new effective catalyst and the improvement of Pt interface for effective reaction site are very important. In addition, in order to increase the current density, it is needed to supply protons, electrons, and oxygen molecules to the Pt surface smoothly, rapidly, and uniformly. In other words, to improve the platinum utilization, the structures of the catalysts should be optimized with various types of materials that are involved in the mass transport pathways. Moreover, an improved mass transport flux in the catalyst layer offers the possibility of increasing the current densities, which in turn allows a reduction in the cell areas,

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