Design of ordered-catalyst layers for polymer electrolyte membrane fuel cell cathodes

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In polymer electrolyte membrane fuel cells (PEMFCs), because the reaction rate in the cathode is slower than that in the anode, the cathode catalyst layers require more catalyst loading than the anodes [1]. Much research has been focused on improving the catalytic activity in cathodes and simultaneously reducing the amount of Pt supported by carbon black, which is the most commonly used cathode catalyst [2-4]. Recently, carbon nanotubes [5-9], carbon nanohorn [10], and carbon nanofibers [11-13] have been developed for Pt support materials for PEMFC cathodes, due to their high electronic conductivity and/or high catalytic activity of the oxygen-reduction reaction. For the catalyst-layer structure, ordered structures have higher potential than disordered structures, yielding improved cell performance due to oriented mass transport [9]. The design of ordered-catalyst layer structures with optimized carbon nanotube alignment, catalyst layer thickness, and proton conductive polymer content is needed to obtain high-performance PEMFCs. In this study, numerical simulations were used to determine the structure of ordered catalyst layers in PEMFC cathodes that yield maximum power density [14].

Ordered catalyst layers were composed of electron conducting tubes with Pt particles on their surface and polymer electrolyte thin films covering on them as shown in Fig. 1.

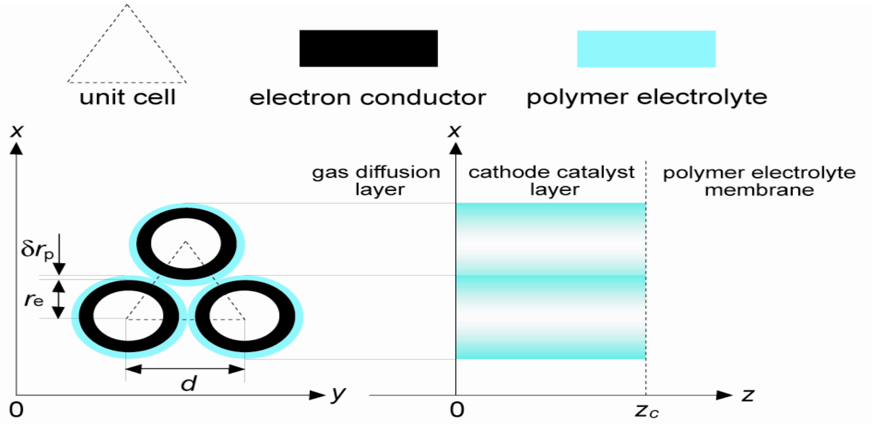

Figure 1 Schematic diagram of an ordered catalyst layer in a PEMFC cathode.

Such catalyst layers were aligned normal to the electrode. The kinetics of oxygen reduction reaction at the catalyst-polymer electrolyte interface and proton and oxygen transport through the polymer electrolyte phase were considered. The catalyst layer structure is similar to Du *et al.* [15], but the difference is that the structural parameters such as the radius of electron conducting tubes, the thickness of the electrolyte film, the distance between the centers of adjacent electron conducting tubes, and the thickness of cathode catalyst layers are variable, and these parameters are optimized to yield maximum power density. A theoretical model based on the agglomerate model [16, 17] was developed to analyze the transport and reaction phenomena inside catalyst layers.

Calculation results showed that at high Pt loading, when the catalyst layer thickness is large and the flux is small, (i) the cell performance is only weakly sensitive to the Pt loading, (ii) the ordered structure must be optimized to obtain the maximum cell performance, and (iii) either reducing the size of the ordered structure or increasing the area ratio of reaction sites to the outer surface of the electron conducting tubes, A_1 has the same effect on cell performance. However, at low Pt loading, when the catalyst layer thickness is small and the flux is large, (i) the cell performance is sensitive to the Pt loading, (ii) electron conducting tubes should be located as densely as possible, and (iii) the size reduction of the ordered structure is essential to improve cell performance.

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