Microscopic analysis of interlayer structure and oxygen transport behaviors in porous electrode in PEMFC

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Multilayered porous electrodes which are composed of catalyst layer (CL), micro-porous layer (MPL) and gas diffusion layer (GDL) are used in proton exchange membrane fuel cells (PEMFCs). These layers are conventionally regarded as homogeneous layers in numerical simulations. However, actual layers can be inhomogeneous because of their surface morphology and large scale gap. This inhomogeneous structure can be an additional resistance for mass transport in the electrode. P. Deevanhxay et al. showed water accumulation at the interlayer of the electrode by soft X-ray spectroscopy [1]. In this study, the interlayer structure was analyzed by cross-sectional visualization and water and oxygen transport based on the interlayer structure was analyzed by numerical simulation especially focusing on interlayer structure of MPL and GDL.

Carbon-cloth type GDL with MPL (LT-1400-W, E-TEK) was used in this study. Structural analysis of the electrode was performed by scanning electron microscopy (SEM) visualization. Cross-section of the MPL/GDL was formed by using cross-section polishing method [2]. It was revealed that in-plane micro-scale crack was formed at an interface in the multilayered porous electrodes according to through-plane crack in the MPL (Figure 1 (a)). These cracks can be formed in the fabrication process of the MPL because of contraction stress. The interlayer cracks were showed not only in carbon-cloth type GDL but also carbon-paper type GDL (not shown).

Based on these observations, water and oxygen transport in the interlayer was analyzed by lattice Boltzmann method (LBM) with liquid water behaviors taken into account. Applied interlayer structure is shown in Figure 1 (b). Width of in-plane crack (w_{crack}) and pitch of fibers (w_{fiber}) were set as structural parameters. All of the walls in the model are hydrophobic. In the two-phase flow LBM analysis of water transport [3], pores in the MPL were not taken into account and regarded as homogeneous wall because the through-plane crack in the MPL is larger than the pores and liquid water go through the crack preferentially [4]. On the other hand, in the single-phase flow LBM analysis of oxygen transport, the MPL was regarded as space and liquid water distribution obtained from the two-phase flow analysis was taken into account and regarded as a wall. The LBM analyses were performed by using two structures, which are $w_{crack} < w_{fiber}$ and $w_{crack} > w_{fiber}$ (Figure 2). In-plane water accumulation is preferential in the case of $w_{crack} > w_{fiber}$, although through-plane water drainage is dominant in the case of $w_{crack} < w_{fiber}$. Oxygen transport analysis of these cases was performed taking water distribution into account. Water saturation of 20% in GDL including interlayer crack was took in both cases. These results showed that large interlayer crack enhances formation of in-plane liquid water film in the interface, resulting in less oxygen gas transport even though macroscopic water saturation in the GDL is constant. There are reports which say that interface of CL and MPL also has interlayer crack [5,6]. In this interlayer, even smaller crack can affect gas transport significantly because this is the nearest interface to reaction sites.

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Reference

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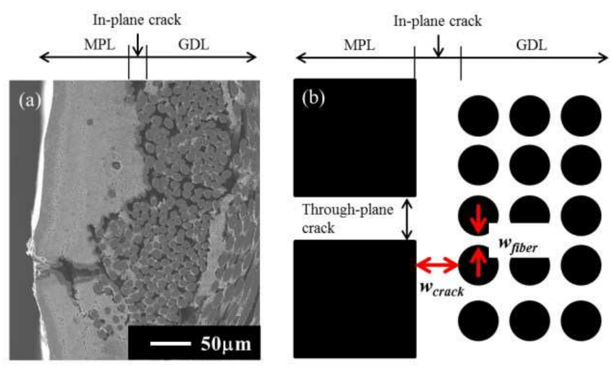

Figure 1. (a) A SEM image of the MPL/GDL cross-section and (b) calculation domain with parameter setting for the simulation.

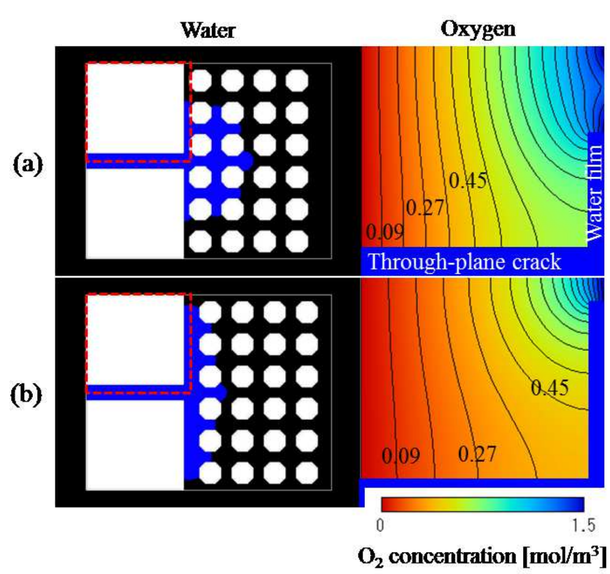

Figure 2. 2D liquid water distribution (left) and contour line of oxygen concentration (right) in the interlayer structure of (a) $w_{crack} < w_{fiber}$ and (b) $w_{crack} > w_{fiber}$ at saturation of 20%. Areas framed by dotted lines in the figures of liquid water distribution are shown in the figures of oxygen concentration distribution.