

Molecular Simulation of Oxygen Permeation Properties through Ionomer on Pt Surface

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Polymer electrolyte fuel cell (PEFC) is expected as a next-generation power source due to its low emission and high efficiency. However, oxygen transport resistance in the cathode side is dominant in the power losses at higher current density [1]. In the cathodic catalyst layer, there are Pt catalysts on supported carbon microparticles, and those particles are covered with ionomer thin films which consist of polymers and water molecules. The ionomer has two properties for the water produce reactions: the proton conductivity and the oxygen permeability. We focused on the oxygen permeation through the ionomer, and molecular dynamics simulations were performed to investigate the water content dependence of the oxygen permeation properties: diffusivity, solubility and permeability [2].

An equilibrium state of the ionomer on Pt surface was constructed as shown in Figure 1, and then oxygen molecules permeate the ionomer. As a result, it is found that the oxygen permeability in the ionomer/gas interface, the bulk region and the ionomer/Pt interface, respectively, decreases as water content increases, and that the oxygen permeability in the ionomer/Pt interface is the smallest. Moreover, comparing the contributions of the diffusivity and solubility of oxygen to the oxygen permeability, the oxygen solubility is dominant in the oxygen permeability in the ionomer.

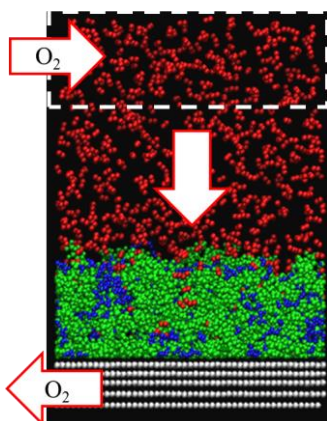


Figure 1 Schematic view of calculation system for oxygen permeation through ionomer on Pt surface.

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