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Molecular Dynamics Studies of Main Factors Affecting Mass Transport Phenomena on Cathode of Polymer Electrolyte Membrane Fuel Cell

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Abstract : In this work, molecular dynamics (MD) simulation is applied to analyze the mass transport process in the cathode of proton exchange membrane fuel cell (PEMFC), of which all types of molecules situated in the cathode is considered. a reasonable and effective MD simulation process is provided, and models were built and compared using both Materials Studio and LAMMPS. The mass transport is one of the key issues in the study of proton exchange membrane fuel cells (PEMFCs). In this report, molecular dynamics (MD) simulation is applied to analyze the influence of Nafion ionomer distribution and Pt nano-particle size on mass transport process in the cathode. It is indicated by the diffusion coefficients calculation that a larger quantity of Nafion, as well as a higher equivalent weight (EW) value, will hinder the transport of oxygen. In addition, medium-sized Pt nano-particles (1.5~2nm) are more advantageous in terms of proton transport compared with other particle sizes (0.94~2.55nm) when the center-to-center distance between two Pt nano-particles is around 5 nm. Then mass transport channels are found to be formed between the hydrophobic backbone and the hydrophilic side chains of Nafion ionomer according to the radial distribution function (RDF) curves. And the morphology of these channels affected by the Pt size is believed to influence the transport of hydronium ions and, consequently the performance of PEMFC.

Keywords : cathode catalytic layer, mass transport, molecular dynamics, proton exchange membrane fuel cell
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