

MERIT Internship Program Report

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Period

September 11th, 2017 – October 27th 2017

Host Company

Toyota Motor Company

Abstract

About a month and a half, I joined the internship at Toyota Motor Company in Toyota City, Aichi Prefecture. I was assigned to Material Creation & Analysis Dept. Material Platform Engineering Div., which studies computer simulation for fuel cell. During this internship, I engaged in analyzing theoretically diffusion mechanism of oxygen in ionomer included in catalyst layer of fuel cell.

Research Activities

Fuel cells are expected to be clean and high efficient energy resource. The key concepts for developing fuel cells for vehicles are “downsizing” “high output” and “cost reduction”. The core of fuel cells is membrane electrode assembly (MEA) composed of a proton exchange membrane and catalyst layer. To get high output, the important things are to increase “catalytic activity”, “proton conduction” and “oxygen diffusion” in ionomer. In this internship, to increase oxygen diffusion in ionomer we performed classical molecular dynamics to analyze the mechanism of oxygen diffusion in ionomer, especially Nafion, which has been heavily used and of which experimental data is rich.

We checked the validity of the calculation model by comparing the theoretical and experimental values of diffusion coefficient. Then, through visualization of diffusion process and quantifying structure of Nafion, we found a key evidence to clarify the diffusion mechanism and pick structure

metrics that can relate to the diffusion process. These results can be applied to increase the speed of calculation for diffusion process and to design new ionomer with higher diffusion coefficient.

Acknowledgement

I would like to thank TOYOTA motor company, especially Director Kume, Chief Takahashi, Ishikura-san, Kimura-san for fruitful discussion. I owe a debt to my supervisor, Prof. Tsuneyuki for permitting to leave the laboratory for long time. Finally, I am grateful for MERIT Program and PCoMS giving me the precious opportunity.