Molecular Dynamics Simulation of Proton Diffusion in Sulfonated Polymer Membranes

James C. Moller[1]

Department of Mechanical and Manufacturing Engineering; Miami University
Oxford, OH 45056

and

Rajiv J. Berry[2]

Polymer Branch; Air Force Research Laboratory
Dayton, OH 45433

[1]Speaker; [2]Corresponding Author (rajiv.berry@wpafb.af.mil)

Introduction

Among the pressing needs for proton exchange membrane fuel cell performance are higher operating temperatures and higher proton mobility. Sulfonated polythioethersulfone (SPTES) polymers have shown promise due to their high proton conductivity and high degradation temperature. In this work, molecular dynamics simulations were conducted to study and compare structures and transport among hydrated Nafion and SPTES.

Results and Discussion

The dependence of the glass transition temperature of the dehydrated polymer on the degree of sulfonation was studied. These results served to verify the force fields used. These fields included descriptions of protonated water and deprotonated sulfonate groups.

Proton diffusion was modeled by both transport on hydronium molecules as well as hopping among hydronium and water. Various strategies for calculating hopping probability were applied. Segregation and ordering among sulfonated groups, the backbone, and water were studied as a function of temperature. The morphology of water/polymer interfaces was also compared.