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Conformational structures in dry ionomers[1] ELSHAD ALLAHYAROV, PHILIP TAYLOR, Case Western Reserve University — The molecular architecture of polymer electrolyte membranes (PEM), which consist of hydrophobic and hydrophilic segments, leads to its own self-assembled structure through a partial phase segregation. Controlling these structures is necessary for improving the performance of fuel cells. We have used computer simulation to analyze the relationship between the hydrophilic cluster structure and the parameters describing the pendant side chains in dry Nafion-like materials. We investigate the morphology of a dry PEM system within different coarse-grained models: a free-proton model, a dipolar model for side chains, and a branched-chain model. We conclude that the free-proton model, where the proton-proton correlations are decoupled from the sulfonate-sulfonate correlations, has the potential to explain the experimentally observed conformational structures of PEM. We find that the geometry of domains with a high concentration of sulfonate groups depends only weakly on the form of the distance-dependent dielectric permittivity, but strongly depends on the partial charge and monomeric unit sequence distribution along the ionomer chain. We predict a nanophase separation with a lamellar-like morphology in ionomers carrying a divalent salt.

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