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Simulation study of proton transport in ionomers[1] PHILIP TAYLOR, ELSHAD ALLAHYAROV, Case Western Reserve University — Coarse-grained molecular-dynamics simulations were used to study the morphological changes induced in a Nafion-like ionomer by the imposition of a strong electric field. We observe that proton transport through this polymer electrolyte membrane is accompanied by morphological changes that include the formation of structures aligned along the direction of the applied field. The polar head groups of the ionomer side chains assemble into clusters, which then form rod-like formations, and these cylindrical structures then assemble into a hexagonally ordered array aligned with the direction of current flow. For dry ionomers, at current densities in excess of 1 A/cm^2 these rod-like clusters undergo an inner micro-phase separation, in which distinct wire-like lines of sulfonate head groups are accompanied by similar wire-like alignments of bound protons. The clusters appear to be of two types. If there are two, four, or five lines of sulfonates then there is an equal number of lines of protons, but if there are three lines of sulfonates then they are accompanied by four lines of protons. Occasionally these lines of sulfonates and protons form a helical structure. Upon removal of the electric field, the hexagonal array of rod-like structures remains, but the microphase separation disappears below the threshold current of 1 A/cm^2.

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