Correlation between structure and conductivity in stretched Naﬁon

ELSHAD ALLAHYAROV, PHILIP TAYLOR, Case Western Reserve University — We have used coarse-grained simulation methods to investigate the effect of stretching-induced structure orientation on the proton conductivity of Naﬁon-like polyelectrolyte membranes. Recent experimental data on the morphology of ionomers describe Naﬁon as an aggregation of polymeric backbone chains forming elongated objects embedded in a continuous ionic medium. Uniaxial stretching of a recast Naﬁon film causes a preferential orientation of these objects in the direction of stretching. Our simulations of humid Naﬁon show that this has a strong effect on the proton conductivity, which is enhanced along the stretching direction, while the conductivity perpendicular to the stretched polymer backbone is strongly reduced. Stretching also causes the perﬂuorinated side chains to orient perpendicular to the stretching axis. The sulphonate multiplets shrink in diameter as the stretching is increased and show a spatially periodic ordering in their distribution. This in turn affects the distribution of contained water at low water contents. The water forms a continuous network with narrow bridges between small water clusters absorbed in head-group multiplets. We ﬁnd the morphological changes in the stretched Naﬁon to be retained upon removal of the uniaxial stress.

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