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An "Alternating-Curvature" Model for the Nanometer-scale Structure of the Nafion Ionomer, Based on Backbone Properties Detected by NMR KLAUS SCHMIDT-ROHR, Q. CHEN, Ames Laboratory and Department of Chemistry, Iowa State University, Ames, IA — The perfluorinated ionomer, Nafion, which consists of a $(\text{-}CF_2\text{-})_n$ backbone and charged side branches, is useful as a proton exchange membrane in H_2/O_2 fuel cells. A modified model of the nanometer-scale structure of hydrated Nafion will be presented. It features hydrated ionic clusters familiar from some previous models, but is based most prominently on pronounced backbone rigidity between branch points and limited orientational correlation of local chain axes. These features have been revealed by solid-state NMR measurements, which take advantage of fast rotations of the backbones around their local axes. The resulting alternating curvature of the backbones towards the hydrated clusters also better satisfies the requirement of dense space filling in solids. Simulations based on this "alternating curvature" model reproduce orientational correlation data from NMR, as well as scattering features such as the ionomer peak and the $I(q) \sim 1/q$ power law at small q values, which can be attributed to modulated cylinders resulting from the chain stiffness. The shortcomings of previous models, including Gierke's cluster model and more recent lamellar or bundle models, in matching all requirements imposed by the experimental data will be discussed.

Klaus Schmidt-Rohr
Ames Laboratory and Department of Chemistry
Iowa State University, Ames, IA

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