Network Formation and Ion Conduction in Ionomer Membranes

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We present the functionalized Cahn-Hilliard (FCH) energy, a continuum characterization of interfacial energy whose minimizers describe the network morphology of solvated functionalized polymer membranes. Charged groups at the surface of solvent-functionalized polymer interface drive the creation of interface through their desire for solvation shells and the reduction of electrostatic free energy. With a small set of parameters the FCH characterizes bilayer, pore-like, and micelle network structures. The gradient flows derived from the FCH describe the interactions between these structures, including the merging and pinch-off of endcaps and formation of junctions central to the generation of network morphologies. Figure 1 depicts three different classes of network structures arising from the FCH gradient flow from initial data and different parameter values. We couple the FCH gradient flow to a model of ionic transport which incorporates entropic effects to localize counter-ions, yielding a flow which dissipates a total free energy, and an expression for the excess electrochemical potential which combines electrostatic and entropic effects. We present applications to network bifurcation, reproduction of Small Angle X-ray Scattering data in Nafion, multiphase extensions, including membrane casting and crystallite formation in annealed Nafion.

[1] N. Gavish, J. Jones, Z. Xu, A. Christlieb, K. Promislow, *Polymers* Special issue on Thin Membranes (2012).
[2] N. Gavish, G. Hayrapetyan, Y. Li, K. Promislow, Physica D, 240, (2011) 675-693.

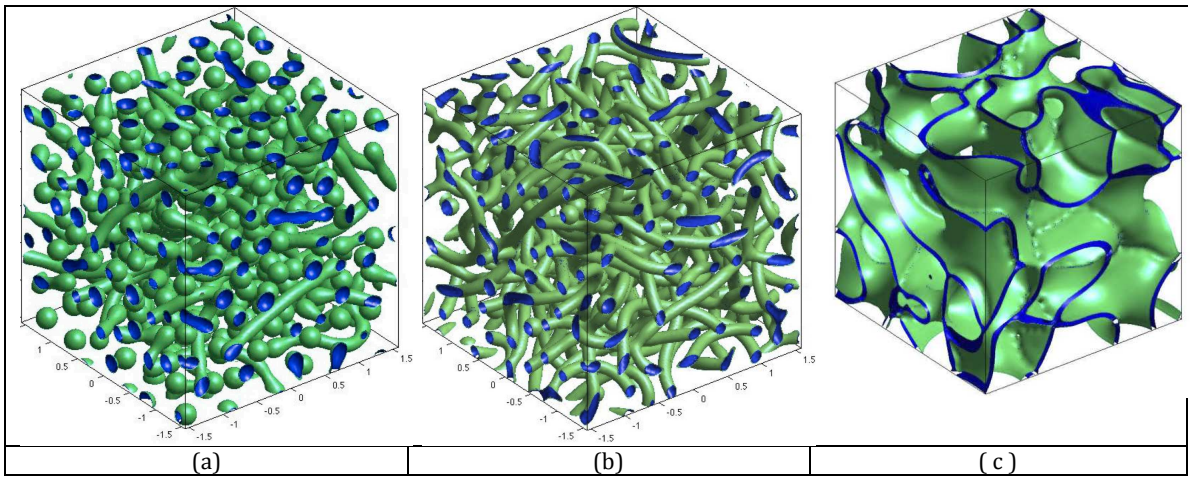

Figure 1: Network morphologies produced from a gradient flow of the FCH energy with three different parameter values, producing (a) micelle, (b) pore, and (c) bilayer dominated networks.