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Multiscale molecular simulations of the formation and structure of
polyamide membranes created by interfacial polymerisation

Large scale molecular simulations to model the formation of polyamide membranes have been carried out using a procedure that mimics experimental interfacial polymerization of trimesoyl chloride (TMC) and metaphenylene diamine (MPD) monomers. A coarse-grained representation of the monomers has been developed to facilitate these simulations, which captures essential features of the stereochemistry of the monomers and of amide bonding between them. Atomic models of the membranes are recreated from the final coarse-grained representations.

Consistent with earlier treatments, membranes are formed through the growth and aggregation of oligomer clusters. The membranes are inhomogeneous, displaying opposing gradients of trapped carboxyl and amine side groups, local density variations, and regions where the density of amide bonding is reduced as a result of the aggregation process. We observe the interfacial polymerization reaction is self-limiting and the simulated membranes display a thickness of 5– 10 nm. They also display a surface roughness of 1–4 nm. Comparisons are made with recently published experimental results on the structure and chemistry of these membranes and some interesting similarities and differences are found.

Attached is a nice figure if you need one for PR stuff. (it is an atomistic rendering of a hydrated polyamide membrane)