Self-Consistent Field Modeling of Diblock Copolymers in Selective Solvents

RAGHURAM THIAGARAJAN, DAVID MORSE, Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN 55455 — The purpose of my poster is to study the driving forces behind the self-assembly of a diblock copolymer AB, consisting of a solventphilic block (B) and a solventphobic block (A), in selective solvents (S). Micellar transformations between spherical, cylindrical, and bilayer curvatures for a model system are tracked using self-consistent field modeling, in real space, in the dilute regime. The transition from a concentrated regime, $\phi_{AB} \sim 1$, to a dilute regime, $\phi_{AB} \sim 0$, is studied. Phase portrait for the concentrated regime is generated using periodic self-consistent field modeling. The unbinding transition, as seen in the periodic counterpart of self-consistent field theory, is compared with the transformations observed in the dilute regime. The two phase regions in the dilute regime are mapped out for the inverted phases as well.

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