Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Molecular Simulation of Bicontinuous Phases in Diblock Copolymer Melts FRANCISCO MARTINEZ-VERACOECHEA, FERNANDO ESCOBEDO, Cornell University — Molecular simulations are used to study the stabilization of different bicontinuous phases in diblock copolymer (DBC) melts. The stabilization approach entails attempting to reduce the packing frustration inside the bicontinuous phases nodes by the addition of a "filler" with affinity for the A component. Two different strategies are considered: 1) addition of selective-solvent particles, and 2) addition of homopolymer. Approximate phase boundaries were found via free-energy calculations. A very dissimilar phase behavior is observed upon increasing the amount of the "additive" in the two different strategies. While with the first strategy (i.e., addition of selective solvent) we observed the progression Gyroid (G) $\rightarrow$ Perforated Lamella $\rightarrow$ Lamella $\rightarrow$ Reversed-Gyroid. With the second strategy (i.e., addition of homopolymer) we observed the progression of morphologies G $\rightarrow$ Cylinder $\rightarrow$ Double Diamond (DD) $\rightarrow$ Plumber's Nightmare (P). In both the DD and the P phases, the homopolymer concentrates preferentially in the nodes, suggesting the reduction of the nodes' packing frustration. In addition, a novel morphology was observed, wherein cylinders of two different diameters alternate in a tetragonal packing. The contrasting difference in the phase behavior observed for the two strategies is understood as a consequence of the difference in mixing entropy exhibited by the two additives.

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Date submitted: 15 Nov 2007 Electronic form version 1.4