558c Lattice Monte Carlo Simulations of the Gyroid Phase in Monodisperse and Bidisperse Block Copolymer Systems

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Lattice Monte Carlo (MC) simulations in the NVT ensemble together with a coarse grained model of the block copolymer chains are used to explore the phase diagram of pure diblock copolymer melts. In addition to the classical morphologies, the Gyroid phase is found to be stable in a narrow region of the phase diagram. Evidence of "packing frustration" inside the Gyroid nodes is found by analyzing cross-sections of the Gyroid structure. The use of polydispersity as a way to reduce packing frustration in the Gyroid phase is explored. Longer chains in polydisperse systems are observed to aggregate preferentially inside the nodes. Interestingly, we find that polydispersity can increase the range of temperatures where the Gyroid phase is stable. Finally, the effect of selective nanoparticles in the stabilization of other bicontinuous phases (e.g., Double Diamond and Plumber's nightmare) is elucidated.