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Dynamic and Topological Properties of Lamellar Phases

VAIDYANATHAN SETHURAMAN, VENKAT GANESAN, Department of Chemical Engineering, University of Texas at Austin, Austin, Texas 78712, USA — We investigate the local dynamical and global topological properties of a diblock copolymer system in its lamellar phase. Explicitly, we investigate the heterogeneity in the dynamics and non-Gaussian parameter (α) of different segments in the ordered phase as a function of its distance from the interface for a chain length of $N = 100$. At short time scales, weak heterogeneities are observed for low degree of compositional segregation and the heterogeneities increased for increased interactions between unlike monomers. Monomers near the interface also showed higher α values compared to those away from the interface. We also investigate the entanglements of ordered lamellar phases using molecular dynamics simulations which reveal a reduction in the average entanglement length for increasing χN . We use self consistent field theory calculations to probe the number of topological constraints near the interface. Such calculations showed an increase in the number of constraints near the interface, thus corroborating the results obtained from molecular dynamics simulations.

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