Chain Exchange Kinetics in Diblock Copolymer Micelles: Comparison of Experimental and Simulation Results

ELENA DORMIDONTOVA, CHUN-CHUNG CHEN, Department of Macromolecular Science and Engineering, Case Western Reserve University, Cleveland, Ohio 44106, USA, REIDAR LUND, LUTZ WILLNER, DIETER RICHTER, Institut fuer Festkoerperforschung, Forschungszentrum Juelich, Germany — The exchange of chains between polymeric micelles in equilibrium has been studied experimentally using a novel Time Resolved Small Angle Neutron Scattering technique and modeled using Monte Carlo (MC) simulations. The experiments for PS-PB in alkanes and PEP-PEO micelles in DMF/water solutions revealed a logarithmic time dependence of the exchange kinetics. In the simulations, the time dependence of surviving chains ranges from a single exponential to stretched exponential behavior and is found to be strongly influenced by the chain conformation and escape criteria. In agreement with the experiments, a logarithmic time dependence was found in the MC simulations for an intermediate time range for micelles with a large number of escapable chains from micelle core and low probability of escaping or for micelles with a broader core-corona interface. The MC results suggest that dynamics of conformational rearrangements in a micelle core plays a decisive role in the micelle exchange kinetics.