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Kinetics of chain exchange in diblock copolymer micelles CHUN-CHUNG CHEN, ELENA E. DORMIDONTOVA, Macromolecular Science and Engineering, Case Western Reserve University, Cleveland, Ohio 44106 — Chain kinetic properties in the core of diblock copolymer micelles were studied using Monte Carlo simulations. In order to escape, a polymer chain first has to assume a compact conformation near the surface of the core. In our simulations, we studied the process of conformational changes of the core-forming block before it is ready to escape from a micelle. The radius of gyration or maximum distance of chain monomers from the core-corona interface were used as criteria to assess the compactness of the chain conformation and therefore its readiness to escape. When the chain exchange kinetics is limited mainly by the rate of conformational changes, the survival fraction of the original chains follows stretched exponential behavior. This is in contrast to theoretical predictions of a single activation process for unimer exchange in diblock copolymer micelles. In our simulations, we recover a single exponential behavior of the survival fraction only for the cases of very low escape probabilities. Increasing the width of the core-corona interface while maintaining the same aggregation number makes it easier for a chain to achieve a ready-to-escape conformation. This accentuates the stretched exponential behavior for the survival fraction which in turn shows a nearly logarithmic decay for a considerable portion of the overall time range.

Chun-Chung Chen
Case Western Reserve University, Cleveland, Ohio 44106

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