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Polymer segregation under confinement: Free energy calculations and segregation dynamics simulations JAMES POLSON, LOGAN MONTGOMERY, University of Prince Edward Island — Monte Carlo simulations are used to study the behavior of two polymers under confinement in a cylindrical tube. We measure the free energy F as a function of the separation of the centers of mass of the polymers λ, and examine the effects of varying the tube diameter D and length L, as well as the polymer length N and persistence length P. For long tubes and fully flexible chains, F monotonically increases with decreasing λ while the chains overlap. The scaling of the free energy barrier height with D and N is close to a prediction using the de Gennes blob scaling model. For finite L, the free energy barrier height increases with increasing L/D at fixed volume fraction ϕ, and it decreases with increasing ϕ at fixed L/D. Increasing the polymer stiffness reduces the overlap free energy. For strongly confined systems, the observed scaling of $F(\lambda)$ with D and P is close to that predicted using a simple analytical model. Finally, MC dynamics simulations are used to study polymer segregation dynamics for fully flexible chains. We find that segregation rates increase with increasing entropic force. In addition, the polymers are not conformationally relaxed at later times during segregation.

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