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The Nanofluidic Staircase: A Brownian Motor for Polymer Characterization and Transport FREDERICK PHELAN JR., National Institute of Standards and Technology (NIST), CHRISTOPHER FORREY, Food and Drug Administration (FDA), JON GEIST, SAMUEL STAVIS, ELIZABETH STRYCHALSKI, National Institute of Standards and Technology (NIST) — A coarse-grained molecular dynamics simulation is used to study the motion of a polymer chain in a nanofluidic staircase (Stavis et al., Nanotechnology, 20(16), 2009), a device which consists of a collection of nanoslits of increasing depth arranged in step-like fashion in a fluidic channel. The slit depths span the Odijk ($H < L_k$) and de Gennes ($L_k < H < R_g$) regimes, where H is the slit depth, L_k is the polymer Kuhn length, and R_g is the radius of gyration. Simulation results show that the model captures the 1-D biased diffusion of chains from regions of high to low confinement that has been measured in recent experiments (Strychalski et al., 14th Int. Conf. on Min. Sys. for Chem. and Life Sci., 2010). The drift velocity increases with increasing step size but also decays more rapidly; stiffer chains drift at a higher rate than softer chains. For all cases, the overall diffusion rates are higher than those calculated for chains in free solution, indicating that the chains gain a "push" as they migrate through the staircase, a manifestation of entropic forces. The staircase system therefore acts as a Brownian motor, which transfers energy from an external source (the polymer free energy) into directed transport using only thermal fluctuations and the biased structural features of the device.

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