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Microsecond MD Simulations of Nano-patterned Polymer Brushes on Self-Assembled Monolayers CREIGHTON BUIE, LIMING QIU, SOYEUN PARK, MARK VAUGHN, KWAN CHENG, Texas Tech University — Nano-patterned polymer brushes end-grafted onto a self-assembled monolayer interface have unique properties and application potential. However, the molecular-level interactions of these brushes with the substrate interface and the solvent are still not clear. Using a coarse-grained MD simulation approach we investigate the structure and dynamics of brushes of monomer length ranging from 25 to 75 units and an implant density σ of 0.2 to 1.0 nm^{-2} that were end-grafted onto a 5×5 nm^2 well in a self-assembled hexadecane monolayer. The behavior of each polymer-monolayer-water complex was simulated from 3 to 12 μs.The excess width and the extended height of the polymers, the nanosecond-resolved conformational transition kinetics from a compact helical to a random coil-like structure, and the time-averaged monomer density maps were determined. The scaling behavior of these brushes differs from that of previous thermodynamic and computational studies of homogeneous brushes and nanopatterned stripes. Here, we find a weaker dependence of brush height on implant density, $\sigma^{0.29}$ rather than $\sigma^{1/3}$ and near linear scaling of the excess width on σ rather than the $\sigma^{1/2}$. Our structural dynamics data and molecular templates are useful for future experimental and computational investigations of nano-patterned polymer brushes at the nanoscopic length and mesoscopic time scales.

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