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Shear-induced desorption of isolated polymer molecules from a planar wall SARIT DUTTA, KEVIN DORFMAN, SATISH KUMAR, Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN — Shear-induced desorption of isolated polymer molecules is studied using Brownian dynamics simulations. The polymer molecules are modeled as freely jointed bead-spring chains interacting with a planar wall via a short-range potential. The simulations include both intrachain and chain-wall hydrodynamic interactions. Shear flow is found to cause chain flattening, resulting at low shear rates in an increased fraction of chain segments bound to the wall. However, above a critical shear rate the chains desorb completely. The desorption process is nucleated by random protrusions in the shear gradient direction which evolve under the combined effect of drag, hydrodynamic interaction, and vorticity-induced rotation, and subsequently lead to recapture. Above the critical shear rate, these protrusions grow in length until the entire chain is peeled off the wall. For free-draining chains, the protrusions are not sustained and no desorption is observed even at shear rates much higher than the critical value. These simulations can help in interpreting experiments on shear-induced desorption of polymer films and brushes.

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