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Brownian Dynamics Simulations of Flow Induced Conformation of Single Polymer Chains ALPARSLAN OZTEKIN, EDWARD WEBB, FRANK ZHANG, XUANHONG CHENG, Lehigh University — Coarse-grained molecular dynamics simulation of single polymer chains is conducted to examine flow induced conformational changes of single polymer chains in shear and extensional flows. Dynamic properties of polymeric molecules are described using bead-spring models; these models put coarse grain groups of atoms into single particles, connected to adjacent particles via spring like interactions. A common representation of the bonded interaction, or spring, is given by the Finitely Extensible Non-linear Elastic model. The constants used in the model are determined form single-molecule force spectroscopic experiments. Simulations and experiments will help to achieve a clear picture of how von Willebrand Factor, a blood clotting protein, model system for flow-induced activation, achieves flow sensing at the single protein/polymer level. The model includes bead-bead interactions, hydrodynamic interaction, the volume of the beads and spring-spring interaction for finitely extensible dumbbell and other spring models. The effects of walls on the dynamics of polymer chains are also presented. The results are presented for various chain lengths and flow conditions. Hydrodynamic interaction and the presence of wall have strong influences on the dynamics of the polymer chain.

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