Molecular dynamic mechanisms of unentangled and entangled linear polyethylene melts in bulk and confined systems under shear flow

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Single molecular chains in bulk and confined systems were categorized into 3 characteristic regimes with respect to the applied flow strength, based on tracking and visualization of simulated systems. In the 1st regime, chain extension and alignment to flow direction began for both systems. Besides to these motions, an interfacial chain alignment on the surface were observed and interfacial entanglements were reinforced for the confined system. In the 2nd regime, the S shape tumbling induced by weak vorticity and disentanglements started for both systems. And also for an interfacial chain, interfacial wagging and interfacial hairpin-like tumbling were detected. In the 3rd regime, a hairpin-like rotation in a tube-like region comprising of highly extended neighboring chains were observed for both systems. Especially, escape of molecular chains from wall and collisions between molecular chains and wall were added for the confined system. Due to the competition between flow field and fluid-wall interactions, interfacial dynamics showed distinctive behavior in comparison to the bulk condition. These microscopic molecular behaviors also were demonstrated with macroscopic and mesoscopic properties.