Mechanism of Interfacial Slip for Polymer Melts using Non-equilibrium Molecular Dynamics Simulation

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Understanding the behavior of interfacial slip is known to play a key role in practical polymer processing, lubrication etc. However, it is challenging to fully understand molecular mechanism of slip. Here, we elucidate the molecular mechanism and dynamics of slip in confined unentangled and entangled linear polyethylene (PE) melts under shear flow. Our results identify three distinctive regimes with regard to the degree of slip (d_s), and reveal the underlying molecular mechanisms. In the weak flow regime, interfacial polymer chains perform the z-to-x rotation in the vorticity plane, which diminishes the wall friction along the flow direction, leading to an increase in d_s. In the intermediate flow regime, the repetitive chain detachment-attachment (out-of-plane wagging) mechanism is found through competition between the flow field and wall interaction, resulting in a constant value of ds for unentangled melts. For entangled melts, d_s decreases with increasing shear rate due to an additional disentanglement mechanism between interfacial and bulk chains. In the strong flow regime, d_s increases again for all systems. This regime is characterized by chaotic chain rotation and tumbling due to collisions between interfacial chains and the wall.