Molecular Characteristics of Stress Relaxation of Polymer Melts upon Cessation of Steady Shear via Molecular Dynamics Simulation

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Stress relaxation after flow cessation is one of the most important nonlinear rheological behaviors for flowing polymeric materials. Considerable researches have been done to examine this phenomenon, but the fundamental molecular characteristics underlying stress relaxation remain unknown. Here, we present detailed molecular mechanisms of the stress relaxation via atomistic nonequilibrium molecular dynamics (NEMD) simulations of the linear polyethylene (PE) melts. We analyze the intrinsic molecular mechanisms behind stress relaxation for entangled polymer systems. It is found that contribution to the stress relaxation seems to be chain conformation-dependent, also subchains along the chains have different relaxation rates. This implies heterogeneous chain relaxation in the system undergoing the stress relaxation. Additionally, to elucidate how entanglement network is formed to reach an equilibrium, entanglement analysis was conducted based on entanglement junctions via the well-known Z1-code. All findings in this study may further help understand other nonlinear phenomena of polymeric systems.