Short Chain Branching Effect on Polymer Structure and Dynamics using Multi-scale Simulations

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A full understanding of chain-branching effects has not yet been established because of a lack of knowledge on the role of short-chain branches, the effects of which have mostly been neglected in favor of the standard entropic-based concepts of long polymers. We performed atomistic nonequilibrium molecular dynamics (NEMD) and mesoscopic Brownian dynamics (BD) under shear flow to investigate a significant role of short chain branching on structural and dynamical properties of polymeric material, and revealed the molecular origins behind the fundamental role of short branches. From simulations and experimental results, we proved that the fast random Brownian motions of short branches plays a crucial role in governing polymer structure and dynamics. Based on our hypothesis on role of short chain branching, we tested various structures of short-chain branched polymers via controlling frequency and arrangement of branches and found intriguing structure-property relations.