Multiscale Simulation of Polymeric Liquids under Flow Conditions

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Polymers have attracted many people's attention for several decades due to the widespread use of polymer products in modern life. In general, polymeric materials undergo numerous processes under various flow conditions to obtain these various polymer products. Therefore, understanding the static (structural and conformational), dynamic, rheological, and topological behavior of polymeric liquids in flowing systems is very significant in polymer processing industry. However, the intrinsic internal complex structure of polymeric materials prevents a fundamental understanding of the static and dynamic behavior of polymer liquids under flow conditions. To facilitate complete understanding on the structure-property-processing relationship of polymeric materials under flow conditions, the hierarchical, multi-level models, such as molecular dynamics (MD), Monte Carlo (MC), Brownian dynamics (BD), and Kremer-Grest (KG) model, were carried out in this study using linear and nonlinear (e.g., branched and ring) polymeric liquids under shear and elongational flow conditions, and were compared with well-established polymer theories (e.g., Rouse and reptation models).