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Tube Dynamics of Mildly Entangled Polymers: Semiflexibility Effects JIAN QIN, SCOTT MILNER, Dept. of Ch. E. at Penn. State Univ., USA, PAVLOS STEPHANOU, Dept. of Math. & Stat. at Univ. of Cyprus, Cyprus, VLASIS MAVRANTZAS, Dept. of Ch. E. at Univ. of Patras, Greece — The prevailing theory of polymer rheology rests on a careful analysis of tube dynamics, tested by comparing predicted rheological response functions to experimental measurements. We provide a direct test of this theory by analyzing the tube dynamics of recently simulated mildly entangled polyethylene melt. The tube dynamics is obtained by defining the tube primitive path, *i.e.*, the tube center line, as the short-time average of molecular dynamics trajectories, and by monitoring how the tangent-tangent correlations evolve with time. It was found that the tube is semiflexible, and that the tube relaxation rate obtained from simulation results cannot be accounted for by the prevailing theory, since the effect of contour length fluctuations built into the theory is too strong. This discrepancy is particularly relevant to the mildly entangled system. To fix this, we incorporated semiflexibility into the theory, which was originally designed for flexible tubes, and found that the corrected theory describes the simulation results nearly quantitatively.

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