Molecular mechanisms of stress overshoot for polymer melts undergoing start-up shear using atomistic simulations

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Stress overshoot is one of the most significant transient behaviors of polymeric liquids undergoing start-up shear at sufficient flow strengths. In spite of substantial previous research effort, fundamental molecular level understanding on stress overshoot remains unresolved. In order to analyze intrinsic molecular characteristic behind stress overshoot phenomena, we performed atomistic nonequilibrium molecular dynamics (NEMD) simulations of lightly entangled linear polyethylene melts under shear flow. Via a detailed analysis of the transient rotational chain dynamics, we found stress overshot occurs through strong intermolecular collisions between chains in the vicinity of the chain orientation angle (20°) with respect to the flow direction corresponding to a peak strain of 2-4, which is an experimentally well-known value.