Fundamental response of ring polymers melts under the shear and elongational flow

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Present dynamic models have been evolved within the range of linear polymers. Unfortunately those models are deficient to study non-linear polymers, especially ring polymers. With the aim of understanding dynamics of ring polymers, we present atomistic nonequilibrium molecular dynamics simulations on unknotted and unconcatenated ring polyethylene melts. C78H156 and C400H800 ring polymers were observed under shear and elongation flows through a direct comparison with the corresponding linear polymers, which have same number of carbons. The structural and rheological responses consistently show that ring melts exhibit considerably lesser degree of deformation against to the applied flow. This is attributed to the intrinsic closed-loop configuration of ring polymers with the constraint that molecules cannot cross each other. As a result, there appears to be a substantial discrepancy between ring and linear systems in terms of chain orientation, the distribution of chain dimensions, viscosity, flow birefringence, hydrostatic pressure, the pair correlation function, and potential interaction energies.