Knotted and unknotted ring polymers under shear

Maximilian Liebetreu and Christos N. Likos

Faculty of Physics, University of Vienna

The behavior of single knotted rings in a fluid under shear is compared to their unknotted ring polymer counterparts. We simulate flexible polymers of a fixed size in a thermostatted Multi-Particle Collision Dynamics (MPCD) solvent (with fixed control parameters) with Lees-Edwards boundary conditions. We primarily investigate the differences in shape parameters for knotted and unknotted rings in dependency of shear rate, as well as characteristics of average number of beads being part of the knot (knot size), angle between knot center of mass and first principal axis relative to the polymer's center of mass, and correlations between quantities. We compute the relaxation time of knotted rings and present results on their tumblingand tank-treading dynamics. We obtain evidence suggesting that on a knotted ring, the knot itself develops a tendency to be located near those beads closest to the orientational axis, aligned with the flow. We also show the average knot size decreasing with increasing shear. Preliminary findings indicate the knotted ring responding to lower shear rates than their unknotted counterparts, and suggest a binary-state behavior for the 31-knotted ring under strong shear, with the knot size alternating between rather stable tight and relatively unstable delocalised configurations. Special attention is paid to the correlation between alignment angle and knot size.