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Influence of Polymer Topology on Polymer Rheology

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Abstract:

In this thesis, we determine the behavior of polymers under shear. To this end, we couple molecular dynamics simulations to the fully-developed hydrodynamic interactions realized by Multi-Particle Collision Dynamics. We introduce an inflation phase exclusive to fully-flexible ring-shaped polymers under shear, which causes a swelling of the ring in vorticity direction and ultimately suppresses tumbling. We derive a theory predicting the shear regime at which inflation occurs. This effect is directly linked to the inclusion of hydrodynamic interactions, highlighting their importance. We investigate the dynamics of knotted rings under shear and determine their similarity to unknotted rings as the knotted section remains well-localized. We study the behavior of semiflexible ring polymers in a nondilute solution and provide evidence that weak shear can be used to re-orient the clusters formed under equilibrium conditions, and that this re-orientation is a long-term effect maintained even after cessation of shear. We determine that cutting a few such rings open, thus turning them into linear chains, does not weaken the clustering behavior observed in equilibrium and also under weak shear, as chains trapped in between clusters provide some additional stability, balancing out the lower effective density of these suspensions. We suggest our findings could be employed in future studies to develop separation methods for linear chains as well as knotted and unknotted rings, to allow predictions about the impact of mixing different topologies in a given system exposed to shear flow, and they could facilitate the development of anisotropic materials with tunable mechanical and transport properties through shear.