Jamming of Knots along a Tensioned Chain

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Massachusetts Institute of Technology — In the limit of very long chains, coiled polymers almost always self-entangle and form knots. In this study, we characterize the motion of these knots along the chain contour when the chain is under very high tension. In this regime, we find that the knot exhibits glassy physics. For example, instead of moving continuously along the contour, the knot becomes kinetically trapped in long-lived, metastable states. This caging phenomenon follows Poisson statistics, and thus the long-time dynamics of the knot are diffusive. We quantify the long-time diffusivity of knots of various topologies, and we find that the diffusivity decays exponentially with increasing chain tension. The rate-of-decay of these transport properties is relatively insensitive to the knot’s topology, which can be explained by examining the energy landscape of the self-reptation moves of the knot along the chain. Finally, we examine the role of bending and excluded volume interactions on this jamming phenomenon. Bending plays the biggest role in determining the onset of jamming, but the corrugation of the excluded volume interactions solely determines the rate-of-decay of the knot’s transport properties.

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