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The diffusion and the size of a knot in a polymer with side chains
LIANG DAI, Singapore-MIT Alliance for Research and Technology, PATRICK DOYLE, MIT — Knots can occur in biopolymers, e.g. DNA and peptides, and synthetic polymers. Polymers often have side chains. We perform Brownian dynamics simulations to investigate the effects of side chains on the diffusion and the size of a knot on a stretched polymer. Three parameters in our model control knots: the length of side chains L_{side}, the gap between two adjacent side chains L_{gap}, and the stretching force f. The knot size L_{knot} is primarily controlled by f. Two distinct regimes are identified. In one regime with $L_{knot} \ll L_{gap}$, the diffusion process is stepwise due to the discrete barriers induced by side chains. In the other regime with $L_{knot} \gg L_{gap}$, the diffusion is continuous and is slowed down due to the friction caused by side chains. The knot size in the small-gap regime changes non-monotonically with the length of the side chain. When the side chain length becomes more than a critical value, the knot shrinks to a small size and rearranged to have side chains outside the knot core to minimize excluded volume interactions. Overall, our results can guide the control of knots by side chains. Furthermore, knotting can be used to investigate molecular friction because knotting ensures significant contact between polymer segments in the knot core.

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