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Force extension response of single self-associating polymer chains

CHARLES SING, ALFREDO ALEXANDER-KATZ, Massachusetts Institute of Technology — The structure and dynamics of polymeric molecules plays a crucial role in a number of synthetic and biological processes. Great progress has been made in using force spectroscopy methods, such as optical tweezers and atomic force microscopy, to probe these properties of single molecules in novel ways. While there has been significant advances at using analytical theory to model the behavior of, for example, single domain unfolding or multi-domain unfolding of identical domains, we consider for the first time the force-extension behavior of self-associating homopolymers. We use a Brownian dynamics simulation with a Bell-like association model that represents, in a coarse-grained fashion, biological polymers such as von Willebrand Factor that use domain-domain interactions to modulate a larger quaternary structure. We also present a theoretical description of pulling that utilizes a master equation description of the relevant coordinate of the polymer network's "shortest chain." We can accurately reproduce the force-extension features, notably the appearance of a dissipative plateau upon the increase of the association time scale, and provide a clear conceptual description of the appearance of this feature. Qualitative comparison to von Willebrand pulling in experiment is shown.

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