Abstract Submitted
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Chains Are More Flexible Under Tension[1] ANDREY DOBRYNIN, JAN-MICHAEL CARRILLO, University of Connecticut, MICHAEL RUBINSTEIN, University of North Carolina — The mechanical response of networks, gels, and brush layers is a manifestation of the elastic properties of the individual macromolecules. The two main classes of models describing chain elasticity include the worm-like and freely jointed chain models. The selection between these two classes of models is based on the assumptions about chain flexibility. We are proposing a unified chain deformation model that describes the force deformation curve in terms of the chain bending constant, K, and bond length, b. This model demonstrates that the worm-like and freely jointed chain models correspond to two different regimes of polymer deformation, and the crossover between these two regimes depends on the chain bending rigidity and the magnitude of the applied force. Polymer chains with bending constant $K > 1$ behave as a worm-like chain under tension in the interval of the applied forces $f \leq KkT/b$ and as a freely jointed chain for $f \geq KkT/b$. (k is the Boltzmann constant and T is the absolute temperature.) The proposed crossover expression for chain deformation is in excellent agreement with the results of the molecular dynamics simulations of chain deformation and single molecule deformation experiments of biological and synthetic macromolecules.

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