

Abstract Submitted
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Tension amplification in branched macromolecules

ALEXANDRU BACANU, JAMES BROCK, University of North Carolina at Chapel Hill, SERGEY PANYUKOV, P. N. Lebedev Physics Institute, MICHAEL RUBINSTEIN, University of North Carolina at Chapel Hill — A molecule's topology can greatly affect the distribution of tension within its bonds. Pom-pom molecules consist of a short linear spacer linking two star polymers, each containing z long arms. The striking ability of this molecular architecture to magnify spacer tension in solution by several orders of magnitude, from the pN to the nN level is due to the steric repulsion between densely packed side chains. In fact, the tension can increase to values that significantly alter the molecule's chemical properties, or even initiate the scission of a carbon-carbon covalent bond in the spacer chain. We study the tension distribution in the spacer and in side branches using molecular dynamics simulations and scaling theory. The dependences of observables such as spacer tension and root-mean-square spacer length on the number of side chains, chemical spacer length, and length of side branches have been quantified. Scaling models are used to explain the interrelated phenomena of tension amplification and spacer elongation and to interpret the results of molecular dynamics simulations.

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