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Quantifying the impact of cyclic defects on polymer network elasticity RUI WANG, Department of Chemical Engineering, Massachusetts Institute of Technology, BRADLEY OLSEN, JEREMIAH JOHNSON, Department of Chemistry, Massachusetts Institute of Technology — Despite the ubiquity of applications, much of our fundamental knowledge about polymer networks is based on an assumption of ideal end-linked structure. However, polymer networks invariably possess topological defects: loops of different orders. Here, we develop a kinetic graph theory which demonstrates the universal cyclic topology of polymer networks. The theory is in excellent agreement with experimental measurements of hydrogel loop fractions without any fitting parameters. The one-to-one correspondence between the network topology and primary loop fraction demonstrates that the entire network topology is characterized by measurement of just primary loops. Different cyclic defects cannot vary independently. To study the correlations between the network topology and gel elasticity, we develop a real elastic network theory (RENT), a modified phantom network theory that accounts for the impacts of cyclic defects. We demonstrate that small loops (primary and secondary loops) have vital effect on the modulus; whereas this negative impact decreases rapidly as the loop order increases, especially for networks with higher junction functionalities. Loop effect can propagate to its neighborhood strands. RENT provides predictions that are highly consistent with experimental observations of polymer network elasticity, providing a quantitative theory of elasticity that is based on molecular details of polymer networks.

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