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Mechanical properties and morphology of polymer gels

YELENA SLIOZBERG, TIMOTHY SIRK, JOHN BRENNAN, JAN ANDZELM, RANDY MROZEK, JOSEPH LENHART, Army Research Laboratory, Aberdeen, Maryland, USA — Understanding morphology and mechanical response of polymeric gels is of particular importance to design materials with required energy dissipation characteristics. We will present our latest results for polymer gels based on 1) self-assembled block copolymers and 2) chemically cross-linked polymers. The dissipative particle dynamics (DPD) was used to predict morphology in good agreement with atomic force microscopy. We have performed DPD non-equilibrium oscillatory shear calculations predicting elastic modulus of unentangled gels that correlates well with experimental rheology data. However, this methodology fails to predict mechanics of entangled polymer networks due to unphysical chain crossing brought by the soft potentials used in DPD simulations. Recently, we have introduced an improved segmental repulsion potential that removes the bond crossing allowing for reptation dynamics. The improved DPD method was used in simulations for entangled gels to explore impact of branched architecture of solvent on the mechanical response to the tensile deformation. Novel architectures of solvent resulting in a dramatic increase of the elastic modulus were identified. The topological analysis was applied to understand contributions of chemical cross-links and entanglements to the stress.

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