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Unified force-level theory of multiscale transient localization and emergent elasticity in polymer solutions and melts ZACHARY E. DELL, KENNETH S. SCHWEIZER, University of Illinois at Urbana-Champaign — A unified, microscopic, theoretical understanding of polymer dynamics in concentrated liquids from segmental to macromolecular scales remains an open problem. We have formulated a statistical mechanical theory for this problem that explicitly accounts for intra- and inter-molecular forces at the Kuhn segment level. The theory is self-consistently closed at the level of a matrix of dynamical second moments of a tagged chain. Two distinct regimes of isotropic transient localization are predicted. In semidilute solutions, weak localization is predicted on a mesoscopic length scale between segment and chain scales which is a power law function of the invariant packing length. This is consistent with the breakdown of Rouse dynamics and the emergence of entanglements. The chain structural correlations in the dynamically arrested state are also computed. In dense melts, strong localization is predicted on a scale much smaller than the segment size which is weakly dependent on chain connectivity and signals the onset of glassy dynamics. Predictions of the dynamic plateau shear modulus are consistent with the known features of emergent rubbery and glassy elasticity. Generalizations to treat the effects of chemical crosslinking and physical bond formation in polymer gels are possible.

Zachary E. Dell
University of Illinois at Urbana-Champaign

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