

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Nonlinear mechanics of thermoreversibly associating dendrimer glasses¹ ARVIND SRIKANTH, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, ROBERT S. HOY, Department of Physics, University of South Florida, BEREND C. RINDERSPACHER, JAN W. ANDZELM, U.S. Army Research Laboratory, Weapons and Materials Research Directorate — The integration of thermoreversibly associating groups into polymers produces a wide variety of complex behavior arising from the finite lifetime of the “sticky,” thermoreversible bonds. Using hybrid molecular dynamics / Monte Carlo simulations, we characterize the nonlinear mechanical properties of associating trivalent dendrimer network glasses with a focus on their energy dissipation properties. Various combinations of sticky bond (SB) strength and kinetics are employed. The toughness (work to fracture) of these systems displays a surprising deformation-protocol dependence; different association parameters optimize different properties. In particular, “strong, slow” SBs optimize strength, while “weak, fast” SBs optimize ductility via self-healing during deformation. We relate these observations to breaking, reformation, and partner switching of SBs during deformation. These studies point the way to creating associating-polymer glasses with tailorable mechanical properties.

¹Funding provided by ARL Contract No. TCN-11042, NSF Grant No. DMR-1263066.

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Date submitted: 08 Nov 2013

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