

Abstract Submitted  
for the MAR16 Meeting of  
The American Physical Society

**Microscopic deformation mechanisms in model thermoplastic elastomers by molecular dynamics simulation** AMANDA PARKER, JÖRG RÖTTLER, University of British Columbia — Thermoplastic elastomers (TPEs) can be formed by exploiting the nanostructured morphology of triblock copolymers. Glassy end-blocks phase separate to form spherical regions which act as physical cross-links for the soft rubbery phase. Molecular dynamics simulations of TPEs allow us to relate the microscopic mechanisms active during plastic deformation to the macroscopic stress response. A coarse-grained bead-spring model of linear ABA triblock copolymers which forms the desired spherical morphology is used for pure stress and pure strain uniaxial deformations. The systems are first equilibrated using a soft pair potential. We observe increased strain hardening in triblocks when compared to homopolymers of the same chain length in accordance with experiments. We connect variations in the stress response for systems of different chain lengths to the non-affine deformation of chains and to the scale of phase separated regions. The stress response is also compared to rubbery elasticity models, taking into account the evolution of chain entanglements during deformation. We observe void formation at the interfaces of glassy regions or where these regions have broken up at large strain.

Amanda Parker  
University of British Columbia

Date submitted: 05 Nov 2015

Electronic form version 1.4