Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Molecular dynamics simulation of a model polystyrene glass[1]
ZHUONAN LIU, SHIQING WANG, MESFIN TSIGE, Univ of Akron — We have performed all-atom molecular dynamics (MD) simulations of a model polystyrene glass to examine such concepts as load-bearing strands (LBSs) and activation zones (AZs) surrounding the LBSs that were proposed in a recent molecular model for yielding and failure of polymer glasses.1 In our simulations, two long chains form a pair of hairpins in a matrix of short polystyrene chains. By deforming the system in different ways including pulling on the two long chains in opposite directions, we examine whether AZs emerge around the two long chains that can be taken as LBSs and how such AZs develop during deformation. 1. S. Wang, S. Cheng, P. Lin, and X. Li, J. Chem. Phys., 2014, 141, 094905.

[1]This work is, in part, supported by NSF grant DMR 144859

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Date submitted: 05 Nov 2015 Electronic form version 1.4