Abstract Submitted
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Chain networking revealed by molecular dynamics simulation YEXIN ZHENG, MESFIN TSIGE, SHI-QING WANG, Department of Polymer Science, University of Akron — Based on Kremer-Grest model for entangled polymer melts, we demonstrate how the response of a polymer glass depends critically on the chain length. After quenching two melts of very different chain lengths (350 beads per chain and 30 beads per chain) into deeply glassy states, we subject them to uniaxial extension. Our MD simulations show that the glass of long chains undergoes stable necking after yielding whereas the system of short chains is unable to neck and breaks up after strain localization. During ductile extension of the polymer glass made of long chain significant chain tension builds up in the load-bearing strands (LBSs). Further analysis is expected to reveal evidence of activation of the primary structure during post-yield extension. These results lend support to the recent molecular model [1] and are the simulations to demonstrate the role of chain networking. This work is supported, in part, by a NSF grant (DMR-EAGER-1444859)

1. S. Q. Wang, S. Cheng, P. Lin, and X. Li, *J. Chem. Phys.*, **2014**, *141*, 094905.

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