

Abstract Submitted  
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**Entanglement Effects in Plastic Deformation of Filled Linear Polymer Glasses**<sup>1</sup> CAMERON ABRAMS, Dept. Chemical and Biological Engineering, Drexel University, DAVID RICHARDSON, Dept. Computer Science, Drexel University — We have performed coarse-grained molecular dynamics simulations of linear polymer glasses with low weight fractions of stiff rodlike particles. This is relevant to understanding the molecular-scale origins of toughness in nanotube-filled polymer composites. Linear polymer glasses are tougher than classical brittle glasses because chains are forced to slide along each other under tensile load to undo entanglements. We focus here on the role of (a) the concentration and (b) orientational distribution of the rod-like inclusion particles on the entanglement network. We observed a substantial (10%) increase in the amount of work required to deform a particular glass plastically to a given strain (2.0) when equal weight fractions of rods were oriented randomly vs. parallel to the pulling axis. Using the method of primitive path analysis [Everaers, et al., *Science* 303:823 (2004)], we identify entanglements and particle-particle bridging interactions which are operative for a given pulling direction in a simulated tensile test in order to predict this enhancement from chain conformations in the initial unstrained sample. We apply this method to many samples with different weight fractions of rods, rod orientations, and rod-polymer interaction strengths.

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