

## **415d Entanglement Effects in the Plastic Deformation of Filled Polymer Glasses: a Simulation Study**

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We have performed coarse-grained molecular dynamics simulations of generic polymer glasses filled with low weight fractions of stiff rodlike particles. The joint hypothesis explored in this project is that the amount of work done in plastically deforming a filled polymer glass is proportional to the number of entanglements that must be “undone,” and that filler particles oriented randomly with respect to an external axis introduce more “operative” entanglements than filler particles oriented parallel to that axis. In a particular simulated tensile test, with a given weight fraction of rods (0.03) and a given molecular weight of polymer (100 “beads”), we observed a 10% increase in the amount of work required to deform the glass plastically to a given strain (2.0) when the rods were oriented randomly relative to the case of rods oriented parallel to the pulling axis. Using the method of primitive path analysis\*, we identify entanglements which are operative for a given pulling direction in a simulated tensile test. We apply this method to many samples with different weight fractions of rods, rod orientations, and rod-polymer interaction strengths. We explore the relationship between the number of such entanglements and (a) the work done in plastic deformation under application of tensile stress in a given direction, and (b) the orientational distribution of the filler rods with respect to that direction.

\*Everaers, et al., Science 303:823 (2004)