MAR07-2006-004759

Abstract for an Invited Paper
for the MAR07 Meeting of
the American Physical Society

Evolution of stress and entanglements during deformation of glassy polymers[1]

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Simulations of the mechanical properties of model polymer glasses have been performed over a wide range of entanglement densities, temperatures, strain rates and chain lengths. Primitive Path Analysis (PPA) is used to examine the corresponding changes in entanglement structure during deformation. Results for the initial yield stress, strain hardening and crazing will be presented. The initial yield stress is a function of strain rate and the thermal history of the sample. Strain hardening can be fit to entropic network models for the stress-strain curve. The stress shows a neo- Hookean response at low entanglement density ρ_e and Langevin strain-hardening at high ρ_e. As expected from network models, entangled polymers deform affinely at scales larger than the entanglement length. However simulations and experiments show strain hardening decreases with increasing temperature while entropic models predict a linear increase. Our results show that strain hardening scales with the flow stress rather than temperature and that substantial strain hardening occurs for unentangled chains. Studies of craze formation show that it does not lead to entanglement loss in our systems. Instead, small scale motions concentrate entanglements at the nodes between fibrils.

[1]Based on work supported by National Science Foundation Grant DMR-0454947