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Abstract for an Invited Paper
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Entanglements and the Mechanical Properties of Glassy Polymers[1]

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The response of glassy polymers to shear or tensile strain is strongly influenced by the entanglement network that is inherited from the melt. Molecular dynamics simulations are used to probe the microscopic origins of stress-strain curves and their connection to entanglements. The latter are identified in real space by examining topological constraints along the primitive path. The first part of the talk will consider the process of craze formation, where the entanglement density is correlated to the volume increase during crazing. Simulations show that entanglements are preserved during crazing, but the craze density does not correspond to pulling chains taut between entanglements. The second part of the talk will examine the effect of entanglements on strain hardening under uniaxial strain. The stress is directly associated with the degree of orientational order along the strain axis, and nearly independent of order along perpendicular directions [1]. Studies with mixtures of short and long chains show that the degree of order is independent of the surrounding chains [2]. The final part of the talk will examine the strength of welds formed by diffusion across polymer interfaces. The shear stress follows the bulk response until chains are pulled taut on the scale of the length of segments that have diffused across the interface. When this length is several times the entanglement length, the maximum shear stress saturates at the bulk value and chains fail through scission. Similar trends are found for the fracture energy in tensile loading.

[1] T. Ge and M. O. Robbins, J. Polymer Sci. B: Polymer Physics **48**, 1473-1482 (2010).
[2] R. S. Hoy and M. O. Robbins, J. Chem. Phys. **131**, 244901 (2009)

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