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Polymer Welding and Self-healing: Strength Through Entanglements[1] TING GE, MARK O. ROBBINS, Johns Hopkins University, DVORA PERAHIA, Clemson University, GARY S. GREST, Sandia National Laboratories — Polymer interfaces are crucial in determining the mechanical strength of many systems. A common means of welding joints or self-healing cracks is to apply heat and allow polymers to interdiffuse. As the microscopic mechanism of interface strengthening is difficult to isolate experimentally, we probe the molecular origins of interfacial strength using large scale molecular simulations of welding and self-healing of cut systems. Systems are heated well above the glass temperature T_g and then quenched below T_g for mechanical testing. The interfacial strength is characterized by the maximum shear stress $\sigma_{\max}$ before failure. As strength grows, the dominant failure mode changes from chain pullout at the interface to chain scission, as in the bulk. In all simulations, $\sigma_{\max}$ saturates long before polymers diffuse by their own size. Bulk strength is observed for miscible welds, while strength is suppressed for cut systems due to short chain segments that remain near the interface. Entanglements are tracked using the Primitive Path Analysis. We find that the bulk response is not fully recovered until the density of entanglements at the interface reaches the bulk value. Moreover, the increase of $\sigma_{\max}$ before saturation is proportional to the number of interfacial entanglements between chains from opposite sides, which correlates linearly with the interdiffusion depth.

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