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**Development of Interfacial Strength and Entanglements During Welding of Polymers** TING GE, MARK O. ROBBINS, Johns Hopkins University, FLINT PIERCE, GARY S. GREST, Sandia National Laboratories, DVORA PERAHIA, Clemson University — Thermal welding is a common means of joining polymer parts. Interfacial strength increases with welding time $t_w$ as polymer chains diffuse across the interface. The microscopic origin of this interfacial strength enhancement was investigated with large scale molecular simulations employing a coarse-grained bead-spring model. Polymer surfaces were held together at a temperature well above the glass transition temperature $T_g$. States at $t_w$ up to $10^9$ time steps were then quenched to a temperature below $T_g$ for mechanical tests. We test the interfacial strength by shearing the weld along a direction parallel to the interface. The maximum shear stress $\sigma_{\max}$before failure is used to characterize the interfacial strength. We find that $\sigma_{\max}$ increases as $t_w^{1/4}$ before saturating to its bulk value. This agrees with previous experiments by a lap-joint shear method [1]. In addition, our analysis shows that the dominant shear failure mode changes from chain pull-out at the interface for small $t_w$, to chain scission for large $t_w$. We examine the average contour length $< l >$ of chains that have diffused across the interface. As predicted by the reptation dynamics, $< l >$ increases as $t_w^{1/4}$. We also track the evolution of entanglements using the *Primitive Path Analysis* (PPA) algorithm [2]. Our results show that the total number of interfacial entanglements is directly related to interfacial strength and also increases as $t_w^{1/4}$.

[1] D. B. Kline, R. P. Wool, *Polym. Eng. Sci.* 1988, 28(1), 52–57.
[2] R. Everaers *et al.* , *Science*, 303, 823-826, 2004

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