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Evolution of Entanglements During Craze Formation TING GE, MARK ROBBINS, Johns Hopkins Univ., ROBERT HOY, Univ. of California, Santa Barbara, STEFANOS ANOGIANNAKIS, CHRISTOS TZOUMANEKAS, DOROS THEODOROU, National Technical Univ. of Athens — Craze formation occurs during fracture of many polymers and leads to a substantial increase in the fracture energy. Models of craze formation usually assume that entanglements act like permanent chemical crosslinks. This model is tested by following the evolution of entanglements using the Contour Reduction Topological Analysis (CReTA) algorithm. The CReTA algorithm shortens each chain until further shortening would require chains to pass through each other. The contacts between chains that limit further shortening are identified as entanglements or topological constraints. Unlike related algorithms, the chain shortening has little effect on the craze structure, allowing the entanglements to be followed in real space, as well as along chains. CReTA is applied to molecular simulations of crazing using a coarse-grained bead-spring polymer model. The number of beads in each chain N and the entanglement length Ne are varied. Our results show that entanglements do not act like fixed chemical crosslinks. There is a systematic loss in entanglements during craze formation that does not occur when chains are deformed affinely and is nearly independent of N/Ne. The role of chain length, N, Ne, interchain friction and other parameters in determining the degree of entanglement loss is discussed.

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