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Welding and healing of polymer interfaces: Connecting structure, dynamics and strength[1]

MARK ROBBINS, Johns Hopkins University

Applying heat to polymer interfaces is a common means of welding polymer components or healing cracks in polymers. Once chains have diffused by their radius of gyration, the properties of the interface should be indistinguishable from those of the bulk. In practice, welds can achieve bulk strength at much shorter times. The mechanism of strength growth is difficult to determine with experiments, because they cannot directly access the evolution of molecular configurations and entanglements. Large-scale simulations were used to follow the dynamics of interdiffusion at welds and cracks and the associated changes in density and molecular conformations.[2] The evolution of entanglements was tracked using Primitive Path Analysis and shown to be directly related to the mechanical strength under shear and tensile loading. As in experiment, the maximum shear strength σ_{max} of a homopolymer interface rises as a power of welding time t and then saturates at the bulk value. Simulations show that σ_{max} is proportional to the areal density of interfacial entanglements at short times and saturates when chains have formed 2-3 entanglements across the interface. Enthalpy limits interdiffusion across heteropolymer interfaces, and there is a corresponding reduction in interfacial entanglements and mechanical strength. A minimum loop length of order the entanglement length must diffuse across the interface to form entanglements. Cracks are more complicated because of the presence of short segments produced during fracture. Segments that are too strong to confer bulk strength, but longer than the entanglement length, remain near the interface for long time intervals. This leads to a plateau in strength that is below the bulk value. Crazes form under tensile loading. A low interfacial entanglement density can stabilize craze formation and significantly enhance the fracture energy, but the bulk fracture energy is recovered at about the same time as bulk shear strength.

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[2]T. Ge, G. S. Grest and M. O. Robbins, ACS Macro Letters 2, 882-886 (2013) T. Ge, F. Pierce, D. Perahia, G. S. Grest and M. O. Robbins, Phys. Rev. Lett. 110, 098301 (2013).