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Interdiffusion and Self-Healing of Entangled Polymer Melts[1]

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The interdiffusion of two polymer films above the glass transition is the simplest way to weld many polymeric materials and is important for self-healing of polymer films which have been torn or damaged. To understand this process better we present molecular dynamics simulations of the interpenetration of two identical homopolymer films described by a bead spring model for the chains with $N = 25$ to 500 beads/chain. As the entanglement length N_e 70, N spans the range from unentangled to highly entangled polymers. For unentangled polymers the mass uptake and penetration depth increase with time t as $t^{1/4}$ for early times crossing over to $t^{1/2}$ for $t > \tau_R$ where τ_R is the Rouse time. For $t > \tau_R$, the mass density profiles are well described by an erf function consistent with classical Fickian diffusion. Entangled polymers also show an extended, early time $t^{1/4}$ scaling for the mass uptake. Unlike the dynamics in a polymer melt which is dominated by the reptation motion of the monomers in the middle of the chain, interdiffusion is found to be dominated by motion of the chain ends, which are known to follow Rouse dynamics.

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