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Possible explanation of anomalous ductility in thermoset/thermoplastic polymer alloys
DEBASHISH MUKHERJI, CAMERON ABRAMS, Drexel University — Mechanical properties of highly cross-linked polymer (HCP) networks, e.g., thermosets, can be significantly modified by adding linear polymer chains, e.g., thermoplastics. In this work, we study thermoset/thermoplastic polymer alloys by means of large scale molecular dynamics simulations (MD) of a coarse-grained model. We focus here on the effect of linear chain mass fraction Γ_l, for different chain lengths N_l, and strain rates $\dot{\varepsilon}$. Our results show that tensile strain (i.e; strain to break) decreases with increasing mass fraction Γ_l, up to a threshold value Γ_l^*, beyond which it increases with Γ_l. This non-monotonic behavior, which we call "anomalous ductility", is qualitatively independent of $\dot{\varepsilon}$ and N_l, so long as fracture occurs in bulk. Γ_l^* decreases with increasing chain length and we observe microscopic evidence that this threshold value signifies the onset of interchain interactions. A simple scaling argument suggests that Γ_l^* is related to the overlap concentration of the thermoplastic homopolymer in the cured thermoset matrix.

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