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Investigation of crazing and cavitation in polymer nanocomposites via simulation GREGORY TOEPPERWEIN, JUAN DE PABLO, University of Wisconsin — Crazing is a unique mode of failure by which polymer strands are stretched into a periodic array of columns. It has been shown that these crazes follow cavitation under deformation. Molecular simulation studies of crazing in nanocomposites have been limited. To explore the connection between nanocomposite structure and some of the local dynamic mechanical effects that are difficult to probe experimentally, we have performed extensive Molecular Dynamics and Monte Carlo simulations of highly entangled polymer nanocomposites with nanoparticles whose size, shape, and concentration have been varied systematically. We investigate the nucleation and growth of voids that precede craze formation to elucidate the role those inclusions play in failure. Calculation of local densities, local stresses and local elastic moduli are used to explain the molecular origins of void formation. The main outcome of our study is a better understanding of how inclusions alter local mechanical properties and how those properties influence failure.

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