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Characterization of pre-mature nanocomposite crazes GREGORY N. TOEPPERWEIN, JUAN J. DE PABLO, University of Wisconsin Madison — 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. Inclusion of nanoparticles drastically alters the glass transition temperature and the globally measurable mechanical properties of these polymer glasses. However, limited literature exists to explain the behavior on the lengths scales of the heterogeneous domains within the glass in the context of nanocomposites. In this work, we investigate the nucleation and growth of voids that precede craze formation to elucidate the role these inclusions play in failure and further characterize the pre-mature craze itself. Extensive Molecular Dynamics and Monte Carlo simulations of highly entangled polymer nanocomposites allow for calculation of local densities, local elastic moduli, and local orientation of additives. We find that the site of void formation is inexorably linked to the local mechanical properties of polymer. This relationship is more evident upon the inclusion of reinforcing additives which induce a broader distribution of local moduli leading to the nucleation of more, smaller voids. Within the developing craze, larger additives resist incorporation, but those that do are subject to ordering.

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