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Mechanical properties of nanocomposite systems GEORGE PAPAKONSTANTOPOULOS, MANOLIS DOXASTAKIS, University of Wisconsin-Madison, MIHAIL VLADKOV, JEAN-LOUIS BARRAT, Universite Claude Bernard (Lyon 1), JUAN DE PABLO, University of Wisconsin-Madison — We employ molecular simulations to investigate the alteration of the mechanical properties upon addition of nanoparticles to a polymer matrix in the melt and the glass regime. In the glass regime, the formation of a stiffer glassy layer is apparent in the vicinity of the nanoparticles. Between particles an increase of the population of local high moduli domains suggests that a second mechanism of property improvement is the formation of a glassy network percolating throughout the material. The distribution of local moduli and the correlation of the non-affine displacements provides interesting insights into the inhomogeneity and the fragility of the nanocomposite and these systems. In the melt regime, relaxation times and viscosity are found to be higher for the nanocomposite systems than the pure polymer. Calculation of chain bridges between the particles is compared to the chain length to examine the bridge formation hypothesis. A primitive path analysis is performed to investigate the effect of inclusions on the entanglement length; results suggest that the entanglement length decreases upon addition of nanoparticles.

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