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Coarse Grain Molecular Dynamics Simulations of the Deformation of Polymer Nanocomposites BARRY FARMER, RICHARD VAIA, KELLY ANDERSON, Air Force Research Laboratory — Nanoscopic dispersions of inorganic nanoparticles in a polymer have been shown to enhance many aspects of the materials performance. Coarse grain molecular dynamics simulations have been used to examine the deformation behavior of these systems. A bead-spring model was used to represent polymer chains and the inorganic layered-silicate phase. The influence of the strength of the interface between the polymer and the layered silicate on the deformation behavior of the nanocomposite has been examined. A weak interface leads to failure between silicate sheets, while for a strong interface, failure occurs in bulk regions of polymer well removed from the silicate. The structure of the deformed material differs from that seen in deformation of the neat polymer.

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