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Physical gelation in polymer-nanofiller systems DI XU, DILIP GERSAPPE, Materials Science and Engineering Department, Stony Brook University, Stony Brook, NY 11790, USA — Polymer gelation by physically crosslinking to sheet-like nanofillers was studied by Molecular Dynamics simulation. Nanofillers were modeled as rigid bodies of disk-like shapes and crosslinks were simulated by introducing a short-range attraction between the nanofillers and polymer chain ends. The structure, dynamics and mechanics of this polymer gel was studied as function of nanofiller volume fraction. Micelle like clusters were formed by polymers wrapping around nanofillers as its cores. These structures grow, with increased filler fraction, into fibrous structures. We observe the formation of a percolated nework of these fibrous structures, with ordered local structure but disordered globally, as we increase the filler fraction. The dynamics of polymers showed significant caging at intermediate time, in gel state, while the polymers move heterogeneously. Stress autocorrelation and elongation results were analyzed as a function of the nano-filler concentration.

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