Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Simulation of Polymer Physical Gel With Platelet Fillers DI XU, DILIP GERSSAPE, Stony Brook University — Platelet filler such as clays have superior effects on the properties of polymer gels. We used molecular dynamic simulations to study platelet filled composite gels system, in which small hexagonal disks simulate the platelets and gelation is due to short-range attraction between end-monomers and platelets. The properties of platelet filled composites are studied as a function of filler concentration. The mechanism of gelation was found similar to those of pure polymer gels; the polymers and platelets formed organic-inorganic networks, which percolate at high enough filler concentration. It was observed platelets aggregated into local intercalation structure, which significantly differs from typical spherical fillers. This unique intercalation structure is examined by radial distribution function and ordering parameters. We discussed how intercalation would affect the properties of the platelet composites by comparing them with spherical fillers.

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Date submitted: 06 Nov 2015 Electronic form version 1.4