Network formation in sheared polymer nanocomposites

EIHAB JABER, HAOBIN LUO, WENTAO LI, DILIP GERSAPPE, Dept of Materials Science and Engg, SUNY at Stony Brook, NY 11794 — We use Molecular Dynamics simulations to study the effects of shear on polymer nanocomposites. Our studies show the formation of a transient network at concentrations exceeding 5% by vol of filler particles. The structure of this network under shear is investigated. We find at lower shear rates the network significantly enhances the viscosity of the polymer, but at higher shear rates it contributes to an acceleration in shear thinning, resulting in a viscosity that is close to the original viscosity of the unfilled polymer system. Our results also show an unexpected effect of fillers on chain orientation under shear. We find that even before a transient network exists in the system, small concentration of filler particles induce a large orientation effect on the polymer chains. Possible implications of this effect will be discussed.

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