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Dissipative Particle Dynamics Simulations of Polymer Nanocomposites NIGEL CLARKE, ARGYRIOS KARATRANTOS, University of Sheffield, RUSSELL COMPOSTO, KAREN WINEY, University of Pennsylvania — We investigate the topological constraints (entanglements) in polymer - nanorod nanocomposites in comparison to polymer melts using dissipative particle dynamics (DPD) simulations. The nanorods have a radius smaller than the polymer radius of gyration. We observe an increase in the number of entanglements, corresponding to a 50% decrease of the entanglement degree of polymerization in the case of 0.11 volume fraction of nanorods dispersed in the polymer matrix, in the nanocomposites as evidenced by larger contour lengths of the primitive paths. The end-to-end distance is essentially unchanged with the nanorod volume fraction for the range of concentrations that we have studied. An increase of the nanorod radius reduces the polymer - nanorod entanglements while the polymer – polymer entanglements remain unaffected. Interaction between polymers and nanorods affects the dispersion of nanorods in the nanocomposites and also alters the primitive path.

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