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Molecular model for the rheology of polymer nanocomposites

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In this work we develop a molecular model for the rheology of entangled monodisperse homopolymers filled with nanoparticles at low filling volume fraction. This research is the continuation of our ongoing effort towards establishing a connection between the macroscopic time-dependent behavior of polymer nanocomposites and their molecular structure. The model is developed based on insight gained from molecular simulations, regarding the structure and dynamics of polymeric chains confined between nanoparticles. These simulations provide physically relevant parameters for the rheological model. The model accounts for reptation, chain stretch and contour length fluctuations. It also accounts for the short-range energetic interactions between polymers and fillers. Its predictions are compared with experimental data. The rheological model is implemented in a FEM package to simulate nanocomposite processing.

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