Abstract Submitted
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Investigation of the Structure and Dynamics of Polyethylene Nanocomposites[1] PETER J. DIONNE, Mechanical, Aerospace and Nuclear Engineering, RAHMI OZISIK, Materials Science and Engineering, CATALIN R. PICU, Mechanical, Aerospace and Nuclear Engineering, Rensselaer Polytechnic Institute — The structure and dynamics of linear, monodisperse polyethylene (PE) melts ($C_{160}H_{322}$ and $C_{440}H_{882}$) containing homogenously distributed spherical nanoparticles were investigated. The PE chains were simulated using a coarse grained model and a Monte Carlo algorithm. Two variables were considered: (i) the wall-to-wall distance between particles (d), and (ii) the interaction energy between monomers and particles. The various chain structures changed greatly with d while the monomer-particle interaction had little effect. The average size, shape, and orientation of PE chains did not differ significantly from those of a neat melt. Bridge segments were more stretched relative to segments in the neat melt and the stretch increased with increasing d. However, the number of bridge segments decreased markedly with increasing d. Chain dynamics was monitored by computing the Rouse relaxation modes and the mean-square displacement of the center of mass. The dynamics were slowed by both geometric effects (confinement by fillers) and energetic effects (monomer-particle energetic interaction).

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