Abstract Submitted
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Diffusion of Trace Alkanes in Polyethylene: Spin-Echo Measurements and Monte-Carlo Simulations[1] E. VON MEERWALL, H. LIN, W.L. MATTICE, University of Akron — We have performed pulsed-gradient NMR diffusion (D) measurements on five n-alkanes (24, 28, 36, 44, and 60 carbons) in a polyethylene (PE) host (M = 33 kDa) as function of concentration c (2-10 wt.%) at 180 deg. C. Monte-Carlo simulations on the second-nearest-neighbor diamond lattice (38, 46, 62, and 78 carbons) at c between 2 and 15 wt.% in a host of PE (M = 4.5 kDa) explored static and dynamic properties. The bridging method uses beads combining adjacent moieties and incorporates two-bead moves; it permits detailed reconstruction of the chain molecules at any stage. It uses discretized short-range rotational isomeric state and long-range intra- and interchain Lennard-Jones potentials. For both experiment and simulation, trace D was obtained by extrapolating D(c) to c = 0 using the Fujita-Doolittle equation with known chain-end free-volume parameters. A ratio of 330 Monte-Carlo steps per picosecond brings simulation into congruence with experiment; this factor is identical to that required for PE melts. The applicability of the Rouse model is approached only for the largest alkanes, but the M(alkane)-dependence of trace D is seen to be in transition from the Rouse-like 1/M-scaling to a steeper value characteristic of reptation with constraint release.

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