

Abstract Submitted  
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**Dynamics of Polyethylene, Studied by Monte-Carlo Simulations<sup>1</sup>**

E. VON MEERWALL, H. LIN, W.L. MATTICE, Univ. Akron — To compare with our diffusion (D) measurements in polyethylene (PE) melts and blends we have performed Monte-Carlo simulations on the second-nearest-neighbor diamond lattice, exploring static and dynamic properties of PE from C40 to C324 (molecular weights M from 584 to 4538) at 180 deg. C. The bridging method is based on beads combining neighboring moieties and now incorporates two-bead moves; it permits detailed reconstruction of the PE chain at any stage. It uses the short-range rotational isomeric state model and long-range intra- and interchain Lennard-Jones potentials as discretized. Reliable results depend on extended prior equilibration. In static properties, chain statistics is non-Gaussian for all but the longest chains, evidenced by an anomalous non-Rouse scaling of  $R_g$  with M; at low M chain-end effects become important. But the autocorrelation functions of the end-to-end vectors still adhere to Rouse and reptation theories for chains longer than C82. Above C100 the relaxation times scale with M in keeping with reptation theory. Center-of-mass D, converted from Monte-Carlo steps to time units according to D measured at a single M, is in excellent agreement with experiment at all M. D of five n-alkanes in M=33k PE extrapolated to trace concentration conforms to the pure Rouse  $1/M$  prediction in the absence of chain-end free-volume enhancements, in good agreement with current experiment.

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