Dynamics of Polyethylene Melts, Studied by Monte-Carlo Methods[1] E. VON MEERWALL, H. LIN, W.L. MATTICE, University of Akron —

In connection with our diffusion measurements in polyethylene (PE) melts we have performed coarse-grained Monte-Carlo simulations on the second-nearest-neighbor diamond lattice to study static and dynamic properties of PE from C40 to C324 (molecular weight M from 584 to 4538). The bridging method is based on beads combining neighboring moieties and now uses two- bead moves; it permits detailed reconstruction of the PE chain at any stage. It uses the short-range rotational isomeric state model and inter- and intrachain Lennard-Jones potentials in their discretized forms. Simulation results become reliable after extended equilibration. For static properties such as the radius of gyration Rg the assumption of Gaussian chain statistics fails for all but the longest chains as Rg scales anomalously with M; at low M chain-end effects become important. But autocorrelation functions of the end-to-end vectors are still interpretable in terms of Rouse and reptation theories for chains longer than C82. Above C100 the relaxation times, converted from Monte-Carlo steps to time units by comparing with experimental diffusion (D) results, scale with M in keeping with reptation theory. At the lowest M, D has a slightly steeper M- dependence than experiment.

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