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Crystal Structures of Precise Functional Copolymers: Atomistic Molecular Dynamics Simulations and Comparisons with Experiments EDWARD B. TRIGG, University of Pennsylvania, MARK J. STEVENS, Sandia National Laboratories, KAREN I. WINEY, University of Pennsylvania — Layered crystal structures have been observed in linear poly(ethylene-co-acrylic acid) in which the carboxylic acid groups are placed precisely every 21 carbon atoms along the backbone. The alkane segments form structures resembling orthorhombic polyethylene crystals, while the acid groups form continuous domains that may act as pathways for ion conduction. Further details of the crystal structure have been difficult to elucidate experimentally, but could be important for understanding structure-property relationships. Here, two classes of crystal structures are evaluated via atomistic molecular dynamics: extended chain structures, wherein the polymer backbones are highly extended in near-trans conformations, and adjacent reentry structures, wherein the polymer backbones conform in adjacent reentry loops near the site of each covalently-bonded acid group. Energies of relaxed structures and hydrogen bonding states are compared, and X-ray scattering and other experimental data is compared with the simulation results.

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