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Simulation of Twist Solitons in Semicrystalline Polyethylene NATHANIEL WENTZEL, SCOTT MILNER, Pennsylvania State University — Semicrystalline polyethylene (PE) consists of ordered lamellae separated by amorphous regions. NMR studies have examined the motion of chains in semicrystalline PE and found that the chains diffuse through the lamellae by propagation of "twist solitons"—localized 180 degree twists of the PE chain. Twist solitons should also be prevalent in PE rotator phases; thermal populations of solitons may play an important role in the free energy of rotator phases, which are stable in oligomeric PE just below melting, and in high molecular weight PE at elevated pressures. We have performed all-atom MD simulations to study the conformations, mobility, and energy of twist solitons in ordered phases of PE, by covalently bonding chains to their periodic image across the periodic boundaries in the z direction. Single twist solitons can be studied in the crystal phase at low temperatures by incorporating a twist in a periodically connected chain, while thermally activated pairs of twists and antitwists are observed at higher temperatures. We speculate that the prevalence of twist solitons in longer alkanes and high molecular weight PE may be responsible for the observed change in chain length dependence of crystal-rotator and crystal-melt transitions above about n=50.

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