

Abstract Submitted
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Molecular Dynamics Modeling of Dielectric Polarization and Ferroelectricity in Poly(vinylidene fluoride) and Related Polymers¹ JEFFREY CALAME, Naval Research Laboratory, Washington, DC 20375 — Molecular dynamics studies of the dielectric polarization response of a constrained bond length and bond angle, united-atom-based model of lamellar crystals of poly(vinylidene fluoride) (PVDF) are reported. Classical ferroelectricity is observed in PVDF, and when variations in the basic PVDF-like interaction parameters are allowed, a transition between classical and relaxor ferroelectricity is found to depend systematically on the polymer repeat unit dipole moment and on the united atom radius of the non-CH₂ functional group. The effects of step and ramp electric field reversal are studied. A complicated sequence of reorientation processes occurs over a wide range of time scales, including a weak, temperature-independent response of 1-2 ps duration associated with local torsional motion, followed by a slow-rising delay regime lasting 10s of ns or longer that involves trans-gauche (TG) transitions in the amorphous phase. After the delay, a large-amplitude primary reorientation occurs over a relatively short additional duration (0.1 to 2 ns), which is due to rotation of large sub-segments in the crystalline phase with few TG transitions. The overall sequence concludes with a slow terminal rise lasting several 100s of ns involving an improvement in crystalline order.

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