Constrained Molecular Dynamics Modeling of Dielectric Response in Polar Polyethylene Analogs and Poly(vinylidene flouride)[1] JEFFREY CALAME, Naval Research Laboratory, Washington, DC 20375 — A simplified molecular dynamics formalism for polymers, having united atoms with constrained bond lengths and bond angles along the backbone but allowing torsional motion, has been developed to model the dielectric response and ferroelectricity in polymers with permanent dipoles. Analytic relations existing on the backbone geometry and associated dihedral motion allow elimination of many dot and cross product evaluations. Also, constraint error correcting forces, symplectic integration with velocity prediction, random force excitation with damping and a momentum-conserving thermostat, and rapid neighbor list and long range force computation allow efficient computation and time steps as large as 20 fs to enable the study of relatively long time scale dielectric phenomena. Studies are performed on non-polar polyethylene for benchmarking, followed by a model system (polar polyethylene) which retains the molecular structure, dihedral potentials, and non-bonded interactions of polyethylene, except artificial partial charges are placed on the united atoms. The modeling is extended to poly(vinylidene fluoride) by changes to the molecular structure, potentials, and charges. Heterogeneous systems containing crystalline and amorphous arrangements of polymer chains are studied.

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