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Temperature dependent structural, elastic, and polar properties of ferroelectric polyvinylidene fluoride (PVDF) and trifluoroethylene (TrFE) copolymers FU-CHANG SUN, AVINASH DONGARE, ALEXANDRU ASANDEI, University of Connecticut, PAMIR ALPAY, Univerisity of Connecticut, SERGE NAKHMANSON, University of Connecticut, UNIVERSITY OF CONNECTICUT TEAM — We use molecular dynamics to calculate the structural, elastic, and polar properties of crystalline ferroelectric β-poly(vinylidene fluoride), PVDF (-CH_2-CF_2-)$_n$ with randomized trifluoroethylene TrFE (-CHF-CF_2-)$_n$ as a function of TrFE content (0-50%) in the temperature range of 0-400 K. There is a very good agreement between the experimentally obtained and the computed values of the lattice parameters, thermal expansion coefficients, elastic constants, polarization, and pyroelectric coefficients. A continuous decrease in Young's modulus with increasing TrFE content was observed and attributed to the increased intramolecular and intermolecular repulsive interactions between fluorine atoms. The computed polarization displayed a similar trend, with the room temperature spontaneous polarization decreasing by 44% from 13.8 μC/cm^2 (pure PVDF) to 7.7 μC/cm^2 [50/50 poly(VDF-*co*-TrFE)]. Our results show that molecular dynamics can be used as a practical tool to predict the mechanical and polarization-related behavior of ferroelectric poly(VDF-*co*-TrFE). Such an atomistic model can thus serve as a guide for practical applications of this important multifunctional polymer.

Fu-Chang Sun
University of Connecticut

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