Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Density functional theory and Molecular Dynamics Studies on Energetics and Kinetics for Electro-Active Polymers: PVDF and P(VDF-TrFE) HAIBIN SU, A. STRACHAN, LANL, WILLIAM GODDARD III, Caltech — We use first principles methods to study static and dynamical mechanical properties of the ferroelectric polymer Poly(vinylidene fluoride) (PVDF) and its copolymer with trifluoroethylene (TrFE). We find that the energy barrier necessary to nucleate a kink (gauche pairs separated by trans bonds) in an all-T crystal is much lower (14.9 kcal/mol) in P(VDF-TrFE) copolymer than in PVDF (24.8 kcal/mol). This correlates with the observation that the polar phase of the copolymer exhibits a solid-solid a transition to a non-polar phase under heating while PVDF directly melts. We also studied the mobility of an interface between a polar and non-polar phases under uniaxial stress; we find a lower threshold stress and a higher mobility in the copolymer as compared with PVDF. Finally, considering plastic deformation under applied shear, we find that the chains for P(VDF-TrFE) have a very low resistance to sliding, particularly along the chain direction.

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Date submitted: 30 Nov 2004 Electronic form version 1.4