Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Multiscale Simulations of Energy Storage in Polymers

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Polypropelene is the most used capacitor dielectric for high energy density storage. However, exotic materials such as copolymerized PVDF and, more recently, polythiourea, could potentially lead to an order of magnitude increase in the stored energy density [1,2]. In our previous investigations we demonstrated that PVDF-CTFE possesses non-linear dielectric properties under applied electric field. These are characterized by transitions from non-polar to polar phases that lead enhanced energy density. Recent experiments [3] have also suggested that polythiourea may be another potential system with high energy-density storage and low loss. However, the characteristics of this emerging material are not yet understood and even its preferred crystalline phases are not known. We have developed a multiscale approach to predicting polymer self-organization using the REAX force field and molecular dynamics simulations. We find that polythiourea chains tend to coalesce in nanoribbon-type structures and prefer an anti-polar interchain ordering similar to PVDF. These results suggest a possible role of topological phase transitions in shaping energy storage in this system.

[1] B. Chu et al, Science 313, 334 (2006).
[2] V. Ranjan et al., PRL 99, 047801 (2007).
[3] Q. Zhang, private communication

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Date submitted: 12 Dec 2011 Electronic form version 1.4