Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Molecular dynamics simulations of electron irradiated PVDF nanofibers[1] JIAYUAN MIAO, Case Western Reserve University, RAM BHATTA, University of Akron, CHRISTIAN KISIELOWSKI, National Center for Electron Microscopy, DINESH LOLLA, DARRELL RENEKER, MESFIN TSIGE, University of Akron, PHILIP TAYLOR, Case Western Reserve University — High-resolution, aberration corrected transmission electron microscopy was used to observe morphological changes and segmental motion of electrospun poly(vinylidene fluoride) nanofibers in an 80 kilovolt electron beam. Atomic and molecular scale high-resolution images of fibers were made with an aberration corrected electron microscope. Chemical and morphological changes, which include the breaking of the fiber, loss of fluorine atoms and cross-linking of chains, caused by the high-energy electron beam were observed. We present the results of molecular dynamics (MD) simulations of such atomic and molecular level observations. The calculational models include the influence of chain scission, chain recoiling, and torsional defects on the morphology of a nanofiber. The effects of the loss of fluorine atoms and the applied tension on the morphology of the fibers were also investigated.

[1]Work supported by the Petroleum Research Fund of the American Chemical Society

Jiayuan Miao
Case Western Reserve University

Date submitted: 12 Nov 2013 Electronic form version 1.4