

Abstract Submitted  
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**Molecular dynamics simulations and morphology analysis of TEM imaged PVDF nanofibers**<sup>1</sup> JIAYUAN MIAO, Case Western Reserve University, DARRELL RENEKER, MESFIN TSIGE, University of Akron, PHILIP TAYLOR, Case Western Reserve University — With the goal of elucidating the structure of polyvinylidene fluoride (PVDF) nanofibers, all-atom molecular dynamics simulations were performed, and the results compared with structures observed in high resolution transmission electron microscopy (TEM) at the molecular level. Simulation shows that the stability of the  $\beta$ -phase component in a PVDF nanofiber is influenced by its thickness and processing history. When exposed to irradiation, as in a TEM observation, the structure is then further modified by the effects of chain scission. The transformation from the  $\beta$  phase into a paraelectric phase can explain the spindle formation and serpentine motion of molecular segments observed by Zhong et al. (Polymer, 54, 2013, 3745-3756) in irradiated PVDF nanofibers. From a comparison between simulated and experimental TEM images it was possible to identify numerous features that are useful in unveiling the inherent structure of PVDF nanofibers. The experimental TEM images appear to match well with those predicted by a model based on  $\alpha$ -phase PVDF, while also being consistent with an alternative model (Nanoscale 2015, DOI: 10.1039/c5nr01619c).

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Philip Taylor  
Case Western Reserve Univ

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