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The Actuation of Semicrystalline Poly(Vinylidene Fluoride) Tie Molecules: A Computational and Experimental Study

Authors : Abas Mohsenzadeh, Tariq Bashir, Waseen Tahir, Ulf Stigh, Mikael Skrifvars, Kim Bolton

Abstract : The area of artificial muscles has received significant attention from many research domains including soft robotics, biomechanics and smart textiles in recent years. Poly(vinylidene fluoride) (PVDF) has been used to form artificial muscles since it contracts upon heating when under load. In this study, PVDF fibers were produced by melt spinning technique at different solid state draw ratios and then actuation mechanism for PVDF tie molecules within the semicrystalline region of PVDF polymer has been investigated using molecular dynamics simulations. Tie molecules are polymer chains that link two (or more) crystalline regions in semicrystalline polymers. The changes in fiber length upon heating have been investigated using a novel simulation technique. The results show that conformational changes of the tie molecules from the longer all-trans conformation at low temperature (β structure) to the shorter conformation (α structure) at higher temperature accrue by increasing the temperature. These results may be applied to understand the actuation observed for PVDF upon heating.

Keywords : poly(vinylidene fluoride), molecular dynamics, simulation, actuators, tie molecules, semicrystalline
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