

Abstract Submitted
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Spectroscopic Analysis of Amorphous Structure in Fluorinated Polymers SHAW L. HSU, YUNING YANG, SURIYAKALA RAMALINGAM, University of Massachusetts Amherst — High-quality polarized Raman spectra have been obtained for various poly(vinylidene fluoride) (PVDF) structures, crystalline and amorphous. These data encouraged us to revisit the Raman band assignment, especially within the conformational sensitive region ($400\text{-}1100\text{ cm}^{-1}$) and use the new understanding to characterize the amorphous region. Vibrational bands have been assigned on the basis of observed polarization characteristics and the calculated potential energy distribution (PED). The simulated results agree well with the experimental polarized Raman study. On the basis of the calculated PED, combined with simulation of different conformational sequences (*tttt*, *tttg*, *tgtg'*, *tggg*, *gggg*), spectroscopic features (band intensity at 648 cm^{-1} and the frequency change of the 856 cm^{-1} band) were associated with the distribution of rotational isomeric states. Two rotational isomeric state (RIS) models were analyzed and compared in the simulation study of the amorphous state. On the basis of the spectroscopic features of experimental and simulated Raman spectra, the conclusion was reached that the model which predicts a higher gauche population more accurately describes the amorphous state. This analysis provides an opportunity to describe the amorphous state in a quantitative manner.

Shaw L. Hsu
University of Massachusetts Amherst

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