Correlation Between Molecular Structure and Dynamics with Opto-Electronic Properties of Poly(9,9-dioctylfluorene-co-benyothiadiazole) - F8BT

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Poly(9,9 '-dioctylfluorene-*co*-benzothiadiazole) (F8BT) is currently one of the most promising material for use as active layers in polymeric electronic devices, such as polymer light-emitting diodes (PLEDs) and field effect transistor (P-FET)[1]. However, as a polymeric material, F8BT exhibit an intricate temperature dependent structure and morphology, making the optoelectronic properties of devices prepared with these materials dependent on temperature, preparation routine, solvent, etc. In this scenario, we present a multi-technique study of the structure, dynamics, and optoelectronic properties of F8BT in order to elucidate the influence of the molecular characteristics in their transport properties. The molecular relaxations of the F8BT films were first investigated by Dynamical Mechanical Thermal Analysis (DMTA) measurements, Differential Scanning Calorimetry (DSC) and ^{1}H Wideline Nuclear Magnetic Resonance (NMR) experiments. The results revealed the presence of two main relaxation process, which occurs at about 225 K (β-relaxation) and 370 K (α - relaxation). A crystalline phase change was also identified by DSC and Wide Angle X-Ray Diffraction (WAXD), occurring at ~ 470 K. The nature of the molecular dynamics that lead to the polymer relaxations were investigated by advanced Solid-State NMR experiments[2]. The results showed that, in the temperature range of 220 to 373 K, the lateral chain execute molecular rotations with average correlation times ranging from 10^{-4} to 10^{-7} seconds. From 300 to 350K the backbone carbons execute slow libration motions with reorientation angles that increase as a function of temperature. Those results were correlated with the changes observed in the Current-Voltage characteristics of thick ITO/F8BT/Al devices in a temperature range of 70 to 490 K. AC measurements as a function of temperature also revealed a strong influence of the molecular relaxations and changes in the crystalline phase on the real impedance. Furthermore, the drift mobility was also measured as a function of temperature using the Time of Flight technique (TOF) and the results show relatively abrupt change on the activation energy of the charge carriers near both relaxations (β and α). Taking all together we show that the electronic states are affected by the molecular processes and present a traping/detraping model that explain mostly of the observed behavior.

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