11th International Conference
on Advanced Materials

Rio de Janeiro Brazil
September 20 - 25

ICAM2009

Effect of Alkali metal salt KCl Doping on Optical and Microstructural Properties of polymer PVA

R. F. Bhajantri[(1)*], V. Ravindrachary[(1)], Ismayil[(1)], A. Harisha[(1)], Manjunath Pattabi[(2)]

(1) Department of Studies in Physics, Mangalore University, Mangalagangotri-574199, India,
(2) Department of Materials Science, Mangalore University, Mangalagangotri-574199, India,
* Corresponding author, e-mail: rbhajantri@yahoo.com

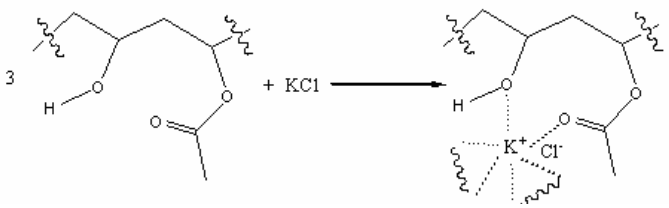
Abstract: The optical, thermal and structural properties of semicrystalline polymer PVA doped with KCl are studied. The FTIR study shows the dopant KCl forms complex with OH/C=O groups of PVA via intra/intermolecular hydrogen bonding. The UV-Visible studies reflect the complex formation, changes the band gap and other optical properties. The XRD result shows the interaction of dopant and complex formation increases the crystallinity due to structural repositioning within PVA. The DSC study indicates the dopant changes thermal behavior of PVA like T_g, T_m and KCl acts as plasticizer. The electrical studies on doped PVA reflect that the doping forms the complex and affects the dc conductivities of PVA.

Doping of polymers attracted the scientific and technological researchers, because of their wide applications. The dopant in polymer can changes the molecular structure and hence the microstructural as well as macroscopic properties of that polymer. Poly(vinyl alcohol) (PVA) has been studied extensively due to its several interesting physical properties which are useful for scientific applications. Various research groups studied the effect of doping on optical, thermal, structural and other microstructural properties of PVA. These studies shows that the properties like crystallinity, structural order, thermal stability, electrical and optical behavior of the polymer are affected by doping which depends on the interaction between the dopant and the polymer [1].

Pure and KCl doped PVA films were prepared from solvent casting method using double distilled water. The FTIR study was carried out using Shimadzu FTIR-8700 Spectrophotometer (400-4000 cm^{-1}). Optical studies were carried out using Secomam Anthelie-284 UV-Vis Spectrophotometer (195-1000nm). The thermal studies of the samples were performed using Shimadzu heat flux DSC-50. X-ray Diffractograms of the samples are conducted using Bruker D8 Advance X-ray diffractometer with Ni-filtered, Cu K_α radiation of wavelength λ=1.5406Á. The DC conductivity studied with Keithley 236 I-V source measure unit.

The FTIR study shows that the dopant KCl forms the complex with OH/C=O groups of PVA via intra/intermolecular hydrogen bonding. The UV-Visible optical studies also reflect the complex formation and affects the original band structure of PVA and changes the band gap as well as other optical properties like shifting of the 206nm peak of pure PVA ($n\rightarrow\pi^*$). Another small peak at 281nm ($\pi\rightarrow\pi^*$) is affected, which comes from unsaturated bonds C=O and/or C=C present in the tail-head of PVA. The presence of dopant and its interaction results in the creation of new molecular dipoles could be a result of point defects created within the band gap. Using the observed UV-Vis spectra, the optical energy band gap E_g is determined by translating the spectra into Tauc's plots. The UV-Visible spectra of pure KCl-water solution shows the absorption edge at 220nm and the estimated optical band gap is 5.63eV, where as for pure PVA it is 4.96 eV. But, when KCl is doped to PVA the optical band gap decreases up to 3.76 eV for 30wt% dopant concentration. The optical activation energy E_t has been estimated using the Urbach formula and the variation in E_t suggests the presence of charge cluster groups i.e. charge transfer complex within the polymer matrix. To get more clear picture on the optical properties of doped PVA the other parameters such as dipole strength (M), transition dipole moment (μ_e), oscillator strength (F) have been estimated [2].

The observed multiple sharp peaks in WAXD spectra in KCl doped PVA indicates the change in crystallinity of PVA. The average crystallite sizes P are estimated using Scherrer's equation which are 5nm for 1wt%, 87nm for 5wt%, 89nm for 10wt%, 96nm for 20wt%, 42nm for 30wt%.The DSC thermograms shows that the T_g and T_m decreases with doping level and hence the KCl is acting as a plasticizer within the PVA. The dc conductivity result shows that the doping forms the complex and presence of such impurities and structural defects results in the trapping of the charge carriers, which enhances the dc conductivity.



[1] R. F. Bhajantri, V. Ravindrachary, A. Harisha, Vincent Crasta, Suresh P Nayak and Boja Poojary, Polymer 47 (2006) 3591.
[2] R M Radwan, J. Phys. D: Appl. Phys. 40 (2007) 374.