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Short Communication

Effect of $BaCl_2$ doping on structural and electrical properties of PEO based solid polymer electrolyte films

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Abstract

$BaCl_2$ doping on structural and electrical properties of Polyethylene Oxide (PEO) polymer electrolyte has studied using FTIR, XRD and conductivity measurements. Pure and doped polymer films were prepared by solution casting method. The chemical modifications within the film due to doping were examined by FTIR study and the result shows that the considerable changes in the doped films, indicates the interaction between dopant and polymer and formation of charge transfer complex (CTC). The XRD study shows the decrease in crystallinity by increase dopant concentration. This shows the presence of CTC modifies the structure of films. The DC conductivity studies show the enhancement of conductivity by increase in BaCl2 salt concentration. The increase in conductivity after 5 wt% ($10^{-6}Scm^{-1}$) has been understood by invoking the CTC behavior within the composite. Conductivity decreases on further addition of salt to PEO polymer electrolyte, which is may be due to the saturation of conducting charge motilities due to doping.

Keywords: Polymer Electrolyte, DC- Conductivity, XRD and FTIR.

Introduction

Solid Polymer electrolytes are one of the resembling stimulating systems in battery applications used in portable devices; several synthetic tactics were accepted to modify the structure, thermal and electrical properties of polymer electrolytes. Among these polymer electrolytes[1], Solid Polymer electrolytes have been quite attractive in development of various applications, from portable electronics to electric vehicles. These have recently been a number of studies on macromolecular design on PEO based solid polymer electrolytes with compressed degree of crystallinity, exhibiting good enhancement in electrical conductivity and improvement in slat solubility. Generally SPE's are the films which possesses transport properties compared to the liquid ionic solutions[2], These SPE's have a vast applications in electrochemical devices like batteries, fuel cells, smart widows, solar cells, etc.

Among the other polymers, PEO polymer electrolyte has been attained various applications due to their mechanical properties, comfort in fabrication at desirable size, Polyethylene oxide is a distinct polymer, it dissolves many varieties of inorganic/ organic compounds to configure polymer electrolytes[3], by adding some inorganic / organic salts, there is a increase in structural and electrical properties of SPE'S. In present study we have discussed about $BaCl_2$ doped PEO polymer electrolytes, the structural and electrical properties are suitably modified by addition of dopant, here the conductivity increases due to degree of crystallinity decreases in polymer composites. In present investigation structural and electrical properties of PEO/$BaCl_2$ electrolyte films were studied.

Materials and methods

Polyethylene Oxide (PEO, molecular weight: 600,000, Sigma Aldrich, USA) and Barium Chloride ($BaCl_2$, Molecular weight: 244.28, Glaxo Mumbai) were used without any further purification. Methanol (CH_3OH, molecular weight: 32.04 g/mol) as a common solvent for the preparation of polymer electrolyte films. Pure PEO and $BaCl_2$ doped electrolyte films were prepared by solution cast technique.

The required amount of PEO and $BaCl_2$ (1%, 3%, 5%, 7% and 10 wt%) were dissolved in 40ml of Methanol solvent and magnetically stirred it for 10-12 hours at room temperature until to get a homogenous solution, the mixture is then poured into cleaned petri dish and kept it for drying at room temperature and allow the solvent to evaporate, after drying the electrolyte film was stored in a desiccators, thickness of electrolyte films are in the range of 0.2-0.3 mm. FTIR, XRD and DC Conductivity studies have been conducted on PEO/$BaCl_2$ complexed polymer electrolytes.

Results and discussion

FTIR studies: In the Figure-1 the chemical group and molecular vibration of pure PEO and PEO doped with $BaCl_2$ is clearly shown that absorption band of pure PEO appearing at around 2990 cm^{-1} to 2740 cm^{-1} represents the C-H stretching modes of CH_2 groups. The width of this absorption band in pure PEO decreases and intensity increases as increase in doping concentration. The CH_2 wagging mode at 1395 cm^{-1} and it shifted 1384, 1372, 1360 and 1359 cm^{-1} in 1,3,5,7 and 10 wt% of $BaCl_2$ complexed films[4]. In the spectral range 1050-1190 cm^{-1} of C-O stretching band, there is decrease in width and intensity of vibration bands are observed in PEO/$BaCl_2$ complexed films. The rest of the bands at around 800-990 cm^{-1} are found to be similar, which are assigned to CH_2 rocking remain unchanged[5].

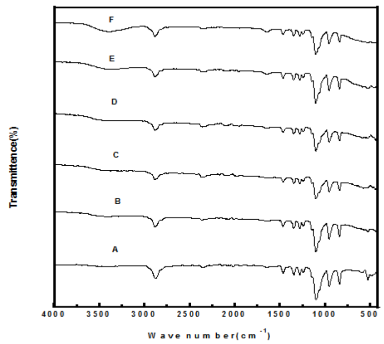

Figure-1: FTIR spectra of (a) Pure PEO (b) PEO + $BaCl_2$ (1%), (c) PEO + $BaCl_2$ (3%), (d) PEO + $BaCl_2$ (5%), (e) PEO + $BaCl_2$ (7%) and (f) PEO + $BaCl_2$ (10%).

XRD studies: The XRD studies examines the modification of crystalline phase by doping different concentration of $BaCl_2$ salt to the PEO polymer, Figure-2 exhibits XRD results of pure PEO, PEO doped $BaCl_2$ film. the diffraction peaks are observed at around $2\Theta = 10^o - 50^o$, The plot of PEO in Figure-2 shows sharp peaks at $2\ \Theta = 19.70^o$ and 23.80^o, the observed crystalline peaks in pure PEO is shifting to lower $2\ \Theta$ values for higher doping level of $BaCl_2$ salt, i.e. $2\Theta = 18.90^o$ and $2\Theta = 23.30^o$ [6], as the dopant concentration increases peak intensity decreases, this shows the degree of crystallinity of polymer electrolyte decreases, which may helps in increase of electrical conductivity. The crystallinity decreases by increase in $BaCl_2$ salt concentration which is clearly exhibited in the Figure-2. i, e The degree of Crystallinity of pure PEO = 0.627387129, PEO/ $BaCl_2$ (1wt %) = 0.56077, PEO/$BaCl_2$ (3 wt%) = 0.547621, PEO/ $BaCl_2$ (5wt %) = 0.509957, PEO/ $BaCl_2$ (7wt %) = 0.422179 and PEO/$BaCl_2$ (10wt%) = 33.58776[7].

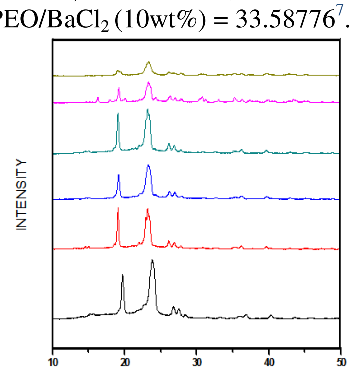

Figure-2: XRD peaks of pure PEO and PEO/$BaCl_2$ (1%, 3%, 5%, 7% and 10%).

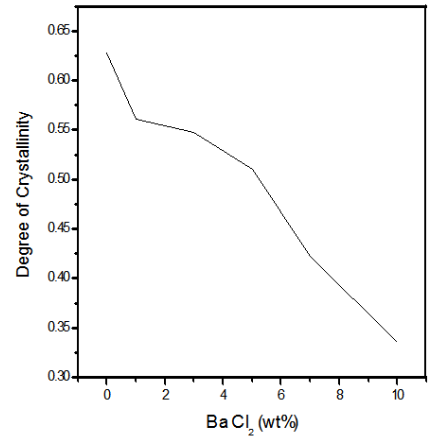

Figure-3: Degree of crystallinity of PEO/$BaCl_2$ of Various concentrations.

DC conductivity: The DC Conductivity at room temperature (RT) is calculated by using below relation,

$$\sigma = \frac{d}{RA} Scm^{-1}$$

Where: d = Thickness of the sample, A = Area of the sample, R = Resistance by slope (average resistance).

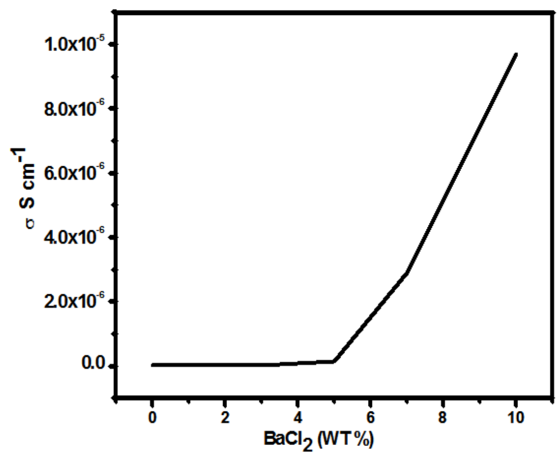

Figure-4: DC Conductivity plot of PEO/ $BaCl_2$ Polymer electrolyte at RT.

The change in conductivity (σ) as a function of $BaCl_2$ wt% is shown in Figure-4. The conductivity increases by increase in salt concentration[8], generally it is believed that the conductivity increases due to decrease in degree of crystallinity of the sample and is discussed in XRD studies[9].

Conductivity of PEO is 10^{-9} S cm^{-1} at RT and it increases as salt concentration increases, it is about ~10^{-8}, 10^{-7} at 1, 3 and 5 wt % of $BaCl_2$ and highest conductivity have been achieved at 7 and 10 wt % of $BaCl_2$ salt doping concentration, which is about ~ 10^{-6} at RT, the increase in conductivity become slower and the sample losses its stability on further addition of $BaCl_2$ salt to PEO Polymer[10].

Conclusion

From this study it is clear that $BaCl_2$ doping affects the structural and electrical properties of Polyethylene Oxide (PEO) polymer electrolyte. The FTIR study shows that the dopant $Bacl_2$ interacts with the polymer and forms the charge transfer complex (CTC). The XRD study shows the presence of this complex due to doping decreases in crystallinity. The DC conductivity studies show the enhancement of conductivity by increase in $BaCl_2$ salt concentration. The increase in conductivity after 5 wt% (I, e.10^{-6} Scm^{-1} at 7 and 10 wt%) is mainly due to the presence of CTC as well as the reduction in the crystalline structure of the composite. Conductivity decreases on further addition of salt to PEO polymer electrolyte, which is may be due to the saturation of conducting charge motilities due to doping.

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