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Studying the effect of KCl Addition on the Optical Properties and Morphological of the Solid Polymer Electrolyte film.

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Abstract: In this work polymer electrolyte based polyethylene oxide doped with potassium chloride films were prepared using the solution cast method. The structural property of doped PEO polymer electrolyte films was examined by XRD. The optical properties of samples are investigated by measuring optical absorption spectra in the wavelength range 190~800nm using UV-Vis spectroscopy and its optical energy band gaps are decreases with increasing the KCl content. The variation in film morphology was examined by SEM.
Keywords: Polymer electrolytes, absorption edge, optical band gaps, XRD, SEM.

1. Introduction

The interest in solid materials with ionic conduction and optical properties has become important during the last few years due to their application in solid state batteries, optical device, sensors and electro chromic devices. Among the polymer, PEO based polymer electrolyte is paid more attention due to its stability, water solubility as well as in inorganic solvent, high capacity in salt complexation, and mechanical flexibility[1,2]. However, the optical properties like reflection, antireflection, interference and polarization should necessary to tune for use in various applications. The optical properties of polymers can be modified by the addition of dopants depending on their reactivity with the host matrix [3]. This technique depends on transition of electron from the valence band to conduction band, when photon energy is greater than the band energy [4,]. This paper report the study of optical properties of PEO based complexes.

2. Experimental Work

10 and 20% KCl doped PEO film was prepared by using the solution cast technique. PEO (M_w=5x10^6) powder was procured from M/s. Sigma-Aldrich, USA, potassium chloride (KCl) from M/s Loba Chemicals (M.W.74.55), and methanol from NICE Chemical. The PEO: KCl of different wt% was dissolved in methanol; the mixture was stirred for about 8h at 303K. The homogeneous mixture was then cast on to a petri dish and allowed to evaporate finally obtain films.

3. Results and Discussion

3.1. XRD Study

X-ray diffraction study was carried out using Rigaku miniflex 600-bench top X-ray diffractometer with CuKα radiation (λ = 1.54178 Å). Fig. 1 shows the X-ray diffractograms of PEO and doped films, the calculated values are presented in table1. It is clearly seen from the fig 1 that intensity decreases with increase the dopant.

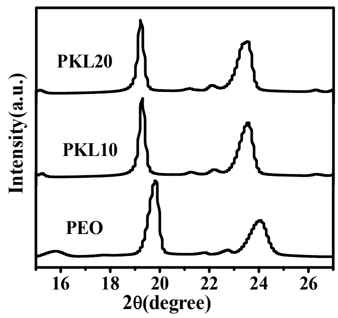

Figure 1 XRD pattern of the pure and doped polymer electrolyte films.

Generally, it is found that the intensity and FWHM increase (0.26-0.28), and then the crystallite size decrease. The average crystallite size has been calculated using the Scherrer formula.

$$L = \frac{k\lambda}{\beta \cos\theta} \quad (1)$$

The average inter-chain separation is calculated using the following equation;

$$R = \frac{5\lambda}{8 \sin\theta} \quad (2)$$

The variation in crystallite size and average inter-chain separation is shown in table 1.
After adding different wt% of KCl, the crystallinity decreases and increase the amorphous, these results agreed well with the obtained SEM results.

Table1: Structural and Optical parameters of PEO and doped polymer electrolyte films.

Films	2θ	d(Å)	β	L (nm)	R(Å)	Direct band Gap(eV)	Indirect Band Gap(eV)	Absorption Edges (eV)
PEO	19.80	4.48	0.4706	17.89	5.59	4.95	3.76	4.62
PKL10	19.30	4.59	0.2620	10.63	5.74	4.75	3.52	4.51
PKL20	19.19	4.62	0.2790	14.71	5.77	4.12	2.96	4.12

3.2. Optical Absorption

The absorption coefficient α (ν) was calculated from the optical absorbance A(ν) after correction for reflections, α (ν) was calculated using the relation

$$I = I_0 \exp(\alpha \ell) \quad (3)$$

where I_0 and I are the incident and transmitted intensities, respectively, and ℓ the sample thickness [5–7]. The relationship between fundamental absorption and optical energy gap is given by the relation

$$E_{opt} = \frac{hc}{\lambda} \quad (4)$$

where c is the velocity of light. At high absorption coefficient levels for non-crystalline materials, the coefficient α (ν) can be related to the energy of the incident photon from

$$(\alpha\ (v)\mathbf{h\nu}) = \boldsymbol{\beta}(\mathbf{h\nu} - E_{opt})^{r} \quad (5)$$

where β is constant and the exponent r an index determined by the type of electronic transition causing the optical absorption and can take values0.5,3/2,2 and 3 for direct allowed, direct forbidden, in direct allowed and indirect forbidden transitions, respectively. When a direct band gap exists, the absorption coefficient has the following dependence on the energy of the incident photon as

$$\alpha \mathbf{h\nu} = \boldsymbol{\beta}(\mathbf{h\nu} - \mathbf{E_{opt}})^{\frac{1}{2}} \quad (6)$$

where α is the absorption coefficient, ν the frequency of the incident light and h the Planck's constant. The optical absorption spectra of pure and doped PEO films are shown in Fig. 2.

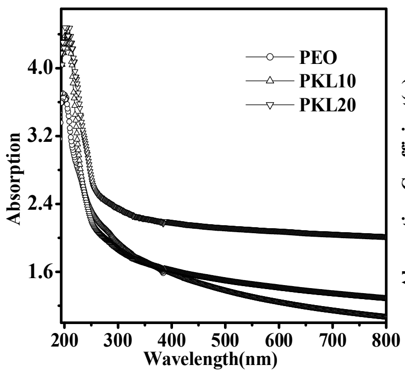

Figure 2 Absorption spectra for PEO/KCl films.

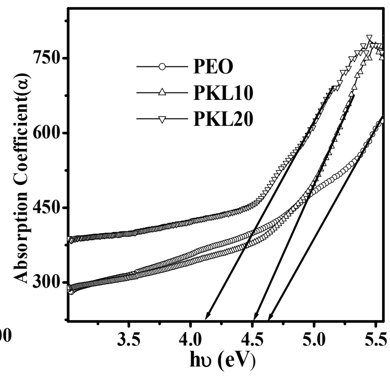

Figure 3 Absorption Coefficients (α) vs photon energy for PEO/KCl films.

To determine the nature and width of the band gap, α, was plotted as a function of photon energy(hν) are shown in Fig.3 and the absorption edge values were obtained by extrapolating the linear portions of the curves to zero absorption value.

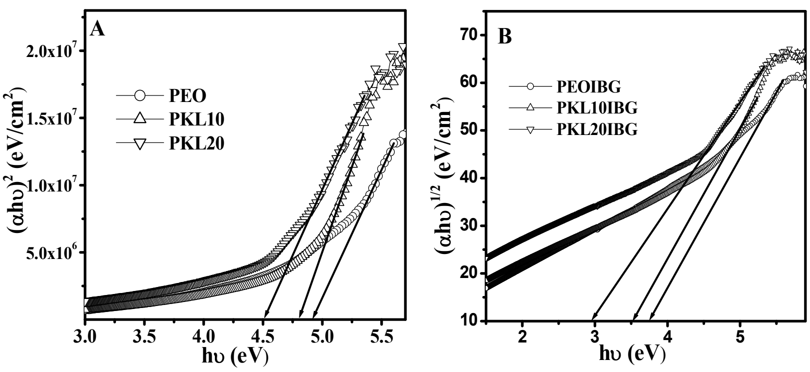

Figure 4| a) $(\alpha h\nu)^2$ and b) $(\alpha h\nu)^{1/2}$)vs. photon energy for PEO/KCl complex.

The optical band gaps were evaluated from $(\alpha h\nu)^2$ vs. hν plots The best fitting to the absorption spectra in Eq.(4) gives r =1/2, meaning the electron allowed direct transition for these composite samples. The allowed direct transition energies were determined by extrapolating the linear portion of Fig. 4 curves to zero absorption and the slope gives the value of constant β . For PEO the direct band gap at 4.95eV, while for 10 and 20 wt% KCl complexes, the values decrease from 4.95 to 4.12eV and it is seen that optical band gaps found decreases with increasing the dopant weight percentage in host polymer system and estimated values are cited in the table 1. The change in band gap could be due to structural changes introduced by doping.

3.3 Surface Morphological Analysis

SEM images of PEO and doped films were obtained by JEOL Model JSM, 6390LV model.Fig.4a–c shows the SEM micrographs for PEO/KCl composites.

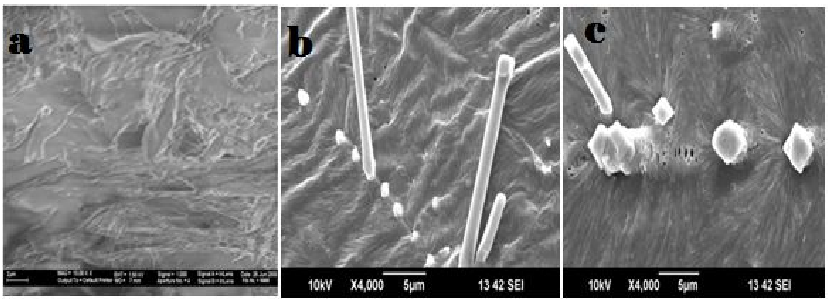

Figure 4 SEM images of (a) PEO, (b) 10 wt %, KCl and (c) 20wt% KCl electrolyte films.

It reveals that different shapes and size of the KCl particles are dispersed in the PEO matrix. It is found that the KCl grain size, roughness is changed. There is considerable modification in the morphology with increasing salt. Fig.4 (a) PEO film is seen that the large spherulite with rough surface, as a doped films particles and small rod like different size structure appear on the surface of the PKL10%.Fig. 4(b) electrolyte film and PKL20% it seems that the particles, rod like different size structure increases increase the dopant concentration and also smoothly surface Fig. 4(c) These changes in the morphology confirm the doping effects on polymer films.

4. Conclusions

PEO/KCl polymer electrolytes have been successfully prepared and the complexation was confirmed by XRD and SEM analysis. The optical energy gaps show a decreasing with increasing the concentration. The direct band gaps of 0, 10 and 20wt% KCl composites were determined as 4.95, 4.75, and 4.50eV, respectively. The spectral dependence of the optical curves indicates that the optical parameters change with dopant effect.

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