

# Structural and Optical Studies of Pure and Iodine Doped Polystyrene Films

K.Maragatham<sup>1</sup> Dr.S.Muruganand<sup>2</sup> N.Manikandan<sup>3</sup>

<sup>1</sup>Research scholar <sup>2</sup>Asst. Professor

<sup>1,2,3</sup>Electronics and Instrumentation Department

<sup>1</sup>Karpgam University,Coimbatore <sup>2,3</sup>Bharathiar University,Coimbatore

**Abstract---** Polystyrene thin films are prepared by solution growth technique using glass substrates. Polystyrene solution is prepared by dissolving 3g of polystyrene in the 100cc of benzene. 1% and 2% iodine doped polystyrene films have been prepared. Pure and iodine thin films are subjected to XRD, FTIR. XRD shows the amorphous nature of thin films. The FTIR spectrum gives about the presence of functional groups in the PS thin films. Also the optical properties polystyrene and iodine doped polystyrene films have been studied.. The optical properties of above thin films have been analyzed using their transmission spectra and the results were discussed. .

**Keywords:** Polystyrene ,iodine,optical, XRD, FTIR.

## I. INTRODUCTION

The science and technology of thin film have made revolutionary changes in microelectronics industries and even today they continue to be recognized globally as frontier area of the research. Thin film technology gains paramount importance since it unravel the complex nature of electronics systems. The obvious reason for preparing materials in the thin film form and studying their properties is that , the two film surfaces are very close to each other and they can have decisive influence on the internal physical properties. The properties differ in a profound way from those of a bulk material[1]. The technical interest in the study of the properties of thin film has resulted in the invention of important devices such as, solar cells, active and passive micro miniaturized components ,magnetic memory devise, reflection and antireflection coating etc.,.

### A. Experimental Techniques

The polymer has long chain and high molecular weight have very complex and considerable variety of physical and chemical structure. Most of the polymer have mixture of polycrystalline and amorphous region, depends on ration of mixture of impurities the strong method is incorporated[2]. The structurally reproducible and pinhole-free film with minimum ageing effects can be produced by the solution growth technique{4-5}.It has explained preparation of polystyrene and iodine doped polystyrene film. Structural and optical property have been studied for the pure and iodine doped polystyrene film.

### B. Solution Growth Technique

The technique used for deposition of thin film in the present study is solution growth, which involves the isothermal immersion of the substrate into the polymer solution of suitable concentration held at a constant temperature for the certain time. The rate of growth and the thickness of the film depends on the nature of the substrate, the concentration,

and temperature of the solution and also on the time for which the substrate is left immersed in the solution.

The polystyrene film were deposited from a polystyrene solution. the solution was prepared by dissolving 3g of PS in 100 cc of benzene. The solution was continuously stirred by means of a magnetic stirrer to ensure a homogeneous mixing. In the same way 0.5%,1% and 2% iodine doped PS film were prepared from 0.5%,1% and 2% iodine concentrated homogeneous solution of 3g PS dissolved in 100 cc of benzene. The film dried in 6hr at constant temperature of 333k.

### C. Sample Preparation

The substrate should also have an appropriate heat conductivity to ensure constant temperature of the surface and sufficient heat removal during the operation of electronics devices. The surface of the substrate should be flat and smooth to form the glass slide used in the study is  $2.5 \times 7.5 \text{ cm}^2$ . The pure and iodine doped polystyrene films were characterized optically by recording the transmittance and absorption of the film to evaluate their absorption coefficient, optical and gap and refractive index values. The optical transmittance and absorption spectra of the films have been recorded in the wavelength range 300nm to 1200nm at room temperature using a UV-VIS-NIR spectrophotometer(UN-1601,shimadzu).

## II. STRUCTURAL STUDIES

The structure of thin films plays a vital role in the nature of thin films and hence in the different physical properties which are utilized for device applications. A number of factors such as, the method of thin film deposition, electrical and thermal conditions of the substrate etc.,.

The XRD is used for the structural analysis. Optical absorption studies are used for the identification of presence of dopants and its role. FT-IR absorption study is a known method for the identification of molecular group present in the pure and doped film from their characteristic frequencies.

### A. X-Ray Diffraction Technique

The X-ray diffraction measurements in the present study have been made with a Riga diffractometre. The characteristic  $K_{\alpha}$  radiation for Cu lies at  $1.5418 \text{ \AA}$  the operating conditions for all the samples were 30KV,15mA.the X-ray diffraction gram of pure of PS 2% iodine doped PS films of average thickness of about  $3.4 \mu\text{m}$ .Fig 1a and I e shows that XRD diffraction of pure and 2% doped PS film.

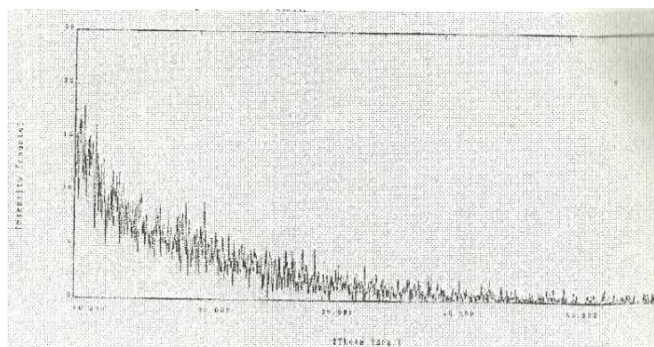


Fig. 1(a): pure PS XRD values

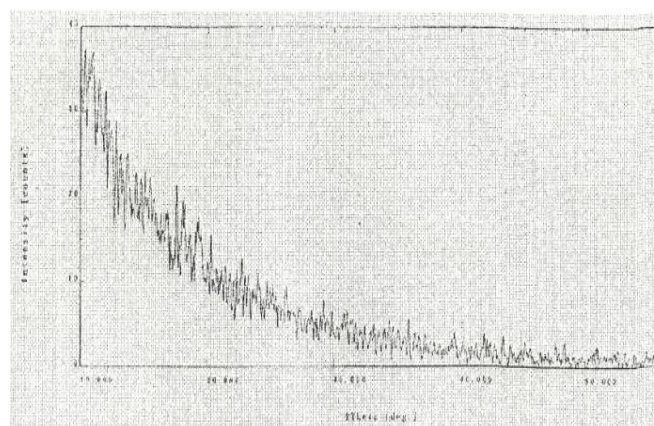


Fig. 1(b): doped Ps , XRD values

Fig (1(a) & 1(b))has describe pure PS and doped Ps , XRD values

**B. Ft-Ir Studies**

The FT-IR spectra of pure PS and 0.5%,1% and 2% iodine doped PS films are recorded using spectrophotometer in the wave number range of (4000-500cm<sup>-1</sup>) . Fig(2a-2d) has been described the FTIR spectra of pure and iodine doped PS film.The absorption band are due to the different stretching and vibration modes of different function group of PS and iodine doped PS. the agreement with the structure of pure PS[8].By comparing the IR spectra of pure and iodine doped PS films from the table .

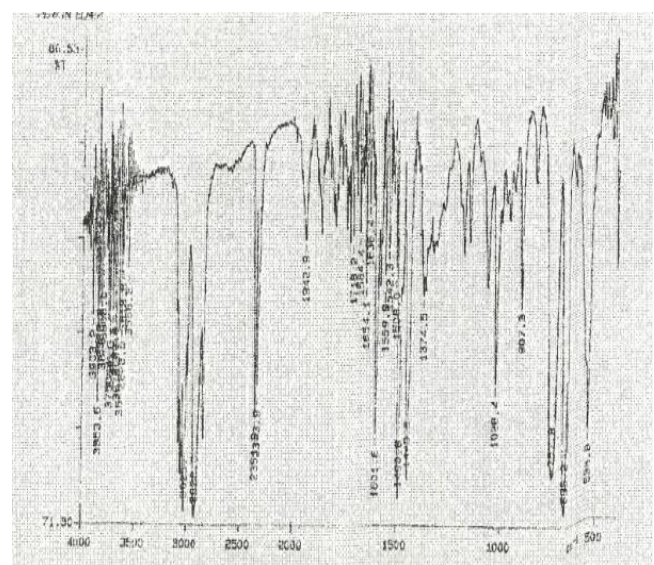


Fig. 2(a): FTIR of pure PS Film

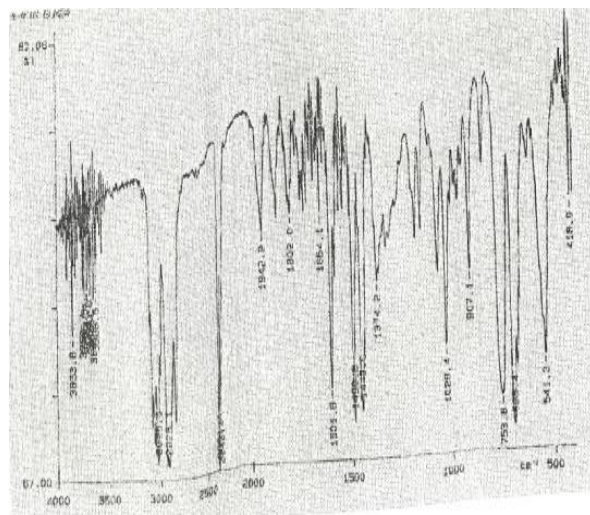


Fig. 2(b): iodine doped PS Film

Undoped PS Film	1% iodine doped PS Film	Assignments
3026.1	3028.4	CH ring stretching
2926.1	2924.1	CH <sub>2</sub> sym.&asym.chain stretching
1490.6	1492.7	CC ring stretching
1449.0	1451.9	CH <sub>2</sub> chain ending
1028.4	1028.4	CH <sub>2</sub> ring plane
753.6	757.3	CH out of plane
695.4	696.8	CH out of plane

Table. 1: comparison

**C. Optical Studies.**

Optical absorption measurements were made in the 200 to 400 nm region at neat normal incidence for pure PS and 0.5% ,1% and 2% iodine doped PS film of 2µm. thickness deposited on glass substrates. In the spectrophotometer has a wavelength range of 190nm to 1100nm with an accuracy of + 3nm.the thickness of the film is 2µm.it has been observe that an additional absorption peak at 200nm has been observed and the breath of the spectrum increased in the case of iodine doped film .the molecular aggregates, which are formed in between the molecular chain of the polymer, impede the movement of charge carriers there by decreasing their mobility.hence absorption peak around 200nm in iodine doped PS has been attributed to either the formation of CTC or molecular aggregates or due to both these formation together whose contribution can be varied by the percentage of doping and temperature/field applied.

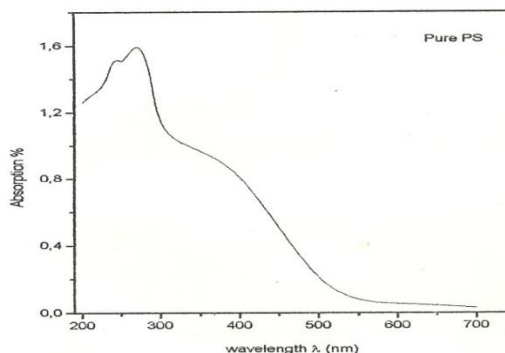


Fig. 3a Absorption % of pure PS film

Fig. 3(a): Absorption % pure PS film

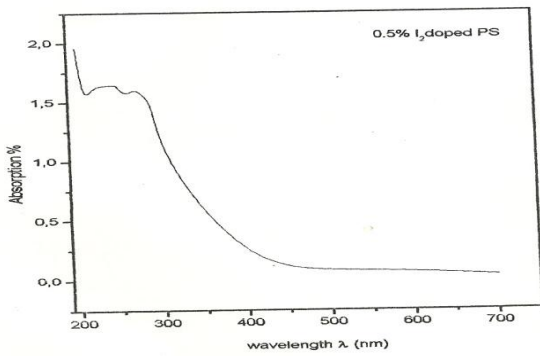


Fig. 3(b) Absorption spectra of 0.5% I<sub>2</sub> doped PS film

Fig. 3(b): Absorption spectra 0.5% I<sub>2</sub> doped PS film  
Fig (3(a)-3(b) has describe the pure and iodine doped PS wave length

### III. RESULT AND DISCUSSION

Films of pure PS and iodine doped PS are found to be highly transparent. the depended of transmission percentage of pure and iodine doped PS film of thickness around 7.4μm on the wavelength of incident electromagnetic radiation ranging from 300nm to 1200nm. It is observed that a small peak is found initially at 400nm and the transmittance percentage increases with length up to 650 nm, beyond it small peak is not present at 400nm as in the case of pure film the transmittance percentage increase with wavelength reaches a maximum and then decreases.

The curve 2%,1% and 0.5% iodine doped PS films shows the maximum transmission percentage as 89.7,89. And 88.9 respectively. The absence of the small peak at 400nm in the case of iodine doped PS films may be due to the presence of iodine and change transfer complex, the transmission has been increasing with the percentage of iodine in PS films.

The optical band gap of the films was determined from the absorption coefficient by fitting the data to the equation[1]  
 $\alpha h\nu = B(h\nu - E_g)^n$

Hv is incident photon energy

B is the edge width parameter

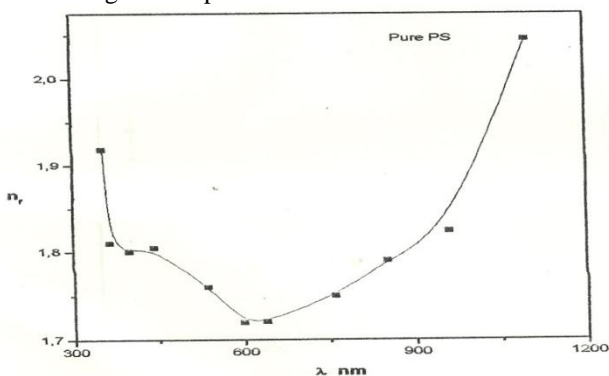


Fig. 4(a): pure PS Kf

And n is the exponent the exponent 'n' determines the type of the electronic transition causing the absorption and can take values 1/2, 3/2, 2 and 3 for direct allowed, direct forbidden, in directed allowed and indirect forbidden transition respectively. The optical absorption data re found to be fit for direct forbidden for exponent n=3/2. The corresponding plot of  $(\alpha h\nu)^{3/2}$  versus hv of the pure and

iodine doped PS film are shown in figures 4(a,b). from the figure 1.a pure PS films is estimated as 1.892eV. the band gap energy values of 0.5% iodine doped PS films were also calculated from the curves of figure 3.a-b as 1.764eV, 1.753eV and 1.630eV respectively.

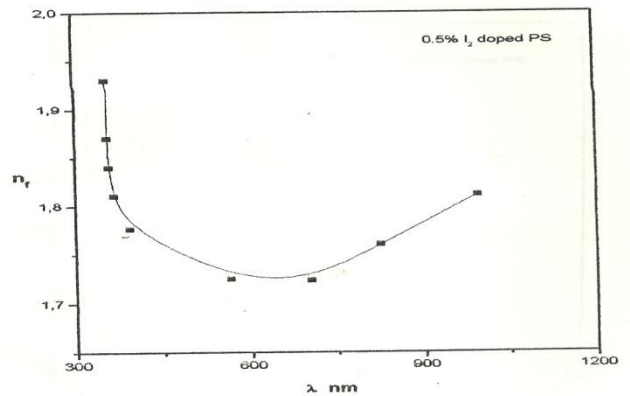


Fig. 4(b): 0.5% iodine doped PS film Kf

The conductivity with increase of doping has been observed in iodine doped poly blend film of polystyrene (PS) and polymethyl methacrylate (PMMA)[4]. As F<sub>6</sub> doped poly (p-penylene) film [5].

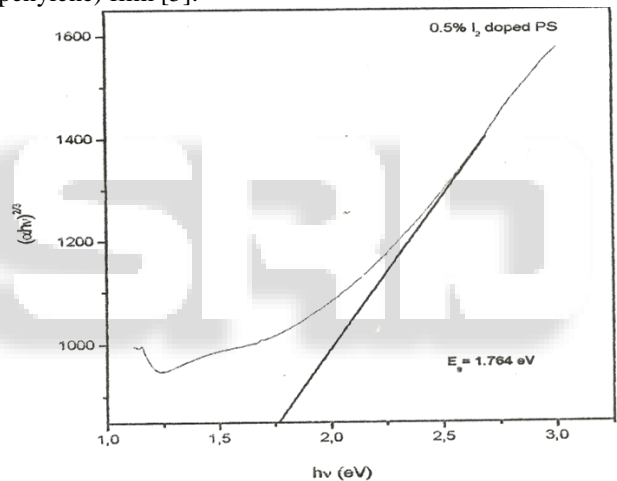


Fig. 5(a): pure PS optical absorption

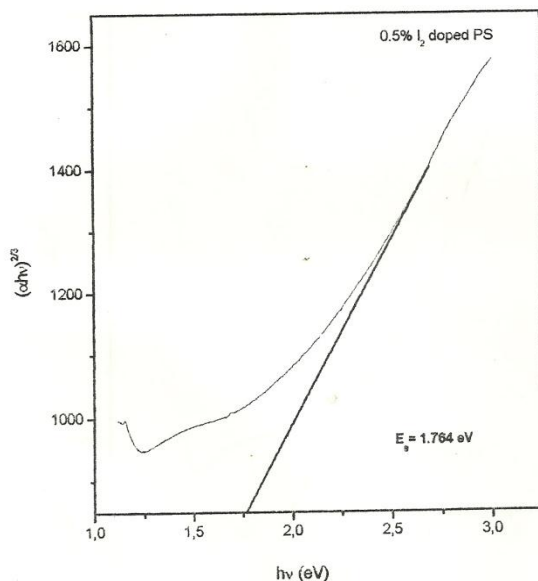


Fig. 5(b): 0.5% iodine doped optical absorption

Fig 5a has described the variation of extinction coefficient( $K_f$ ) values are almost constant up to 600nm for pure film and increase wavelength. It is seen that the values of extinction coefficient is very low for all the films. It is observed that  $K_f$  decreased with increase of iodine doped percentage. The fig 2(a-d) has describe the pure PS and iodine doped PS film wave length( $\lambda$ ) and refractive index( $n_f$ ) for pure and iodine doped PS films plot in diagram. The pure film thickness is  $7.2\mu$ , the refractive index has been increased with increasing of wavelength. In Fig 4b show the plot between the refractive index( $n_f$ ) and wavelength ( $\lambda$ ) for 0.5% iodine doped PS of thickness  $7.15\mu$ , it is observed that the refractive index decreased with increasing wavelength and attain a minimum at 580nm and then increases with increasing wavelength. In the vase of 1% and 2% iodine doped PS film a similar trend is observed and the  $n_f$  value attains the minimum at 500nm, 480 nm respectively, It is noted that the minimum value of refractive index decreased with increase of iodine doping percentage. The observe decrease and increase of refractive index with wavelength may be due to changes in the presence of both amorphous and crystalline phase of varying degrees of crystalline in the film. The changes in the refractive index is and indication of some difference in the bonding ,nearest neighbor distance and dangling bonds[6].

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