

# Spectroscopic analysis of Pure and Ferrocene Doped Polysulfone using X-Ray Diffraction, UV- Visible and FT-IR Techniques

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### Abstract:

In the present study the improvement in dielectric and electrical properties of polysulfone, due to doping of ferrocene was studied. For the study of structural and optical characterization of pure and ferrocene doped foil samples of polysulfone, the spectroscopic analysis techniques like X-Ray diffraction, FT-IR and UV-Visible techniques were used in the present study. The samples of pure and ferrocene doped polysulfone in the form of foil were prepared by isothermal immersion technique. The sensitization of ferrocene was carried out by mixing the 10 mg, 50 mg and 100 mg of ferrocene with 4 gm of pure polysulfone.. The FT-IR characterization study indicates the development of an additional absorption peak at 1407 cm-1 due to doping with ferrocene, whereas other peaks of pure polysulfone remain apparent in doped samples also, but with broadening and gradually reduction in transmittance with the increase of doping ratio. The optical band gap was calculated by UV-visible spectroscopy. In case of UV spectra, out of two absorption regions present in undoped sample, one band merge and only one sharp absorbance peak appears in sensitized samples. It is identified that the UV absorption increases, while band gap decreases with increase in the dopant concentration. The XRD diffractograms of pure and doped samples consists of both sharp and diffused peaks and corresponds to crystalline and amorphous regions respectively. The XRD study confirms structural modification of polysulfone due to change in crystallite size and d-spacing. It was diagnosed that crystallite size and d-spacing decreases with increase in degree of sensitization. The reduction in transmittance of FT-IR peaks, band gap and crystallite size of polysulfone with increase of doping concentration explains a charge transfer complex (CTC) formation between dopant and polymer matrix. These results confirm the improvement of dielectric and electrical properties of polysulfone due to doping of ferrocene.

Keywords: Polysulfone (PSF), Ferrocene, XRD, UV, FT-IR, Charge Transfer

Complex (CTC)

Article History

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#### INTRODUCTION

It has been observed on the basis of previous studies that polymers are a good dielectric materials, as they are capable enough to store charge in them permanently, when subjected to field-temperature treatment. The charge storage capacity of polymers is improved remarkably by impregnating the polymer with suitable dopant. Both inorganic [1] and organic [2] impurities can be used to modify the electrical conductivity of polymers. Inorganic impurities have more profound effects than organic impurities. Dopant molecules generally occupy the interstitial positions between the polymer chains and



link them with some types of bonds due to charge transfer process [19,21]. This reduces the interstitial barriers and increases the transition probability of hopping electrons across these barriers, thus carrier increasing the mobility[19]. Thus impregnation of polymer matrix develops formation of charge transfer complexes (CTCs) between polymer and its dopant. In the past three decades, the considerable development have been observed in the field of electrets made by polymer, which caused the astonishing development of micromachines [3-6]. Considering this point related to enhancement of charge storing capacity of polymer due to doping, Polysulfone is selected as the host polymer and ferrocene as the dopant. It is worthwhile to justify this approach to improve dielectric and electrical properties of polysulfone doped with ferrocene through spectroscopic techniques. In this present study the X-Ray Diffraction, FT-IR and UV-Visible spectroscopic techniques were considered for complete structural and optical characterization of polysulfone pure doped [22]. spectroscopy is used to detect various functional groups present in a material and has been reported as a very useful technique to check the compatibility of host polymer and dopant compound [7].UV-Visible spectroscopy is another tool to observe the changes occurring in optical properties of material after sensitization through absorption peaks. It also provides mathematical support for calculation of direct and indirect band gap [8]. The X-ray diffraction spectroscopy provides valuable information on structural characterization of the selected material. X-Ray diffraction (XRD) is a versatile, non-destructive technique that reveals detailed information about the chemical composition, and crystallographic structure of a crystalline material. It is most widely used for the identification of unknown crystalline materials, and also for the information related to the crystal structure of the films, including lattice constants, crystallite size, phase analysis, crystal defects, stress, etc. [9].In this article, the study of charge transfer

mechanism and development of charge transfer complex (CTC) between polysulfone and ferrocene has been done through spectroscopic analysis by FT-IR, XRD and UV- Visible techniques. It is reported that the formation of CTC between polysulfone and ferrocene improves the dielectric and electrical properties of the polysulfone. This study may lead to polysulfone as a new electret material for designing the solid state devices of large efficiency. In this article, study of all important parameters of spectroscopic studies like transmittance, absorbance, internal chemical structure, crystallite size, spacing between planes, calculation of band gap and refractive index of pure and doped polysulfone have been carried out.

# **EXPERIMENTAL SECTION**Materials

Polysulfone (host): Polysulfone has been utilised in the form of host polymer in this study. Polysulfones belong to the group of thermoplastic polymers. These group of polymers are characterised for their property of toughness and to have stability at elevated temperatures. The subunit represented as aryl-SO<sub>2</sub>-aryl is possessed by them and sulfone group is the specifying component of the said group of polymers. Union Carbide organisation introduced Polysulfones to the world in 1965. Application of Polysulfones, has gained lots of importance in membrane filtration studies specially in 'reverse osmosis'[20]. The reaction of a diphenol bis(4-chlorophenyl) sulfone causes with development of a typical polysulfone. In formation of polysulfone, sodium chloride eliminated, during the reaction of parent compounds. It was reported that during temperature range −100 °C and 150 °C, the properties like rigidness, high-strength, transparency are maintained Polysulfone. The glass transition temperature of polysulfone is 185 °C [10, 11]. The formation of polysulfone compound has been presented in the under mentioned reaction



$$\begin{split} n \; HOC_6H_4OH + n(ClC_6H_4)_2SO_2 + n \; Na_2CO_3 \rightarrow \\ [OC_6H_4OC_6H_4SO_2C_6H_4]_n + 2nNaCl + nH_2O + n \\ CO_2. \end{split}$$

$$\begin{bmatrix} -0 & CH_3 & O & O \\ -CH_3 & O & S & O \\ -CH_3 & O & O \end{bmatrix}_n$$

FIGURE 1. Structure of Polysulfone

**Ferrocene** (**Dopant**): Ferrocene is an organometallic compound, having the formula  $Fe(C_5H_5)^+_{2.}$  The molecule consists of two cyclopentadienyl rings bound on opposite sides of a central iron atom. In this molecule, iron is sandwiched between two cyclopentadienyl rings in staggered conformation, as presented in Figure 2.

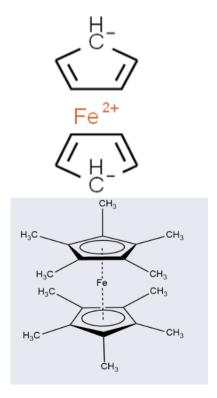


FIGURE 2. Structure of Ferrocene

Ferrocene has been found insoluble in water, but it can be dissolved in organic solvents, like benzene. It remains stable even up to very high temperatures of  $400^{\circ}\text{C}$ . The odor of ferrocene is just like 'camphor' and its colour is 'orange'. Ferrocene is available in solid form , which sublimes above room temperature. Use of ferrocene is recommended due to its exceptional property of stability. It does not decompose even up to heating till  $400^{\circ}\text{C}$  and it remains unaffected by air, water and strong bases. In oxidizing conditions it can reversibly react with strong acids to form the ferrocenium cation Fe  $(C_5H_5)^{+}_{2}$ . To produce carbon nanotubes, Ferrocene can be utilized as a catalyst. [12, 13]

# **Preparation of samples**

**Isothermal Immersion:** The sample was prepared in the 'foil form' and isothermal immersion technique was used for the preparation of the samples [22]. To prepare the pure sample of polysulfone (PSF), its 'beads' were dissolved in solvent dimethylformamide (DMF) .The pure sample of PSF was prepared by liquefying 4 gm of pure PSF in 50 ml of DMF. The mixing of PSF in DMF was done in the glass beaker. To produce the homogeneous and transparent solution of this mixture, mixing was done using a magnetic stirrer at 500 to 700 rpm. Then six number of petridishes of 100 mm diameter are taken. In each of this petridish, sufficient quantity of mercury is poured. About half of the height of the petri dish should be filled with the mercury. Then, in each of these six number of petridishes, glassplates of suitable dimensions are kept. The diameter of the glassplate should be about 80 mm and its thickness should be about 2 mm. The glass plates should be uniform in thickness. The glass plates be properly cleaned, before its use. Then, prepared PSF sample solution was drained (i.e. transferred) over a clean glass plate. This procedure of pouring of PSF sample ,was then repeated for the remaining five number of glass plates, floating on mercury in the petridishes. These glass plates kept on floating on mercury, so that weight of glass plate is equally distributed on



underlying mercury liquid. The care should be taken that petri dishes are kept on truly horizontal surface, so that glass plates are also under truly horizontal position. The mercury is heavier than glass, so it can take the weight of the glass plate. If, instead of mercury, any other lighter liquid like water is used, then glass plate along with overlying sample will be submerged in the liquid. This procedure is also required to be followed, so that the entire surface of the 'foil sample' is of almost uniform thickness. Then all these petri dishes are kept inside in an oven at temperature for around 20 to 24 hours, so that solvent present in the sample is evaporated. The dried sample foils present in petridishes are then taken out of the oven . The glass plates containing sample foils are then slowly removed from the petri dishes. Samples in the form of foil are then carefully removed from the glass plates using sharp cutter etc. The care should be observed that entire circular foil sample should be taken out of the glass plate during peeling process, without getting cut into pieces. Hence, circular foil samples of uniform thickness are

obtained . Doped ferrocene samples of 10 mg, 50 mg and 100 mg in PSF were prepared for the study. For this purpose 10 mg, 50 mg and 100 mg of ferrocene was mixed in the PSF and the same procedure used to prepare pure PSF foil sample was followed. In this way pure PSF samples and PSF samples doped with definite concentration of ferrocene were prepared.

#### RESULTS AND DISCUSSION

Fourier-Transform infrared Spectroscopy (FT-IR): In order to confirm the internal structure of polysulfone (PSF) and to study the chemical reaction between PSF and ferrocene, FT-IR spectrum of pure and doped samples is recorded. It is a steady technique for the identification of various functional groups of materials and to study the mutual chemical interaction between these functional groups of dopant and host polymer matrix. The FT-IR spectrum of pure PSF is presented in Figure 3.

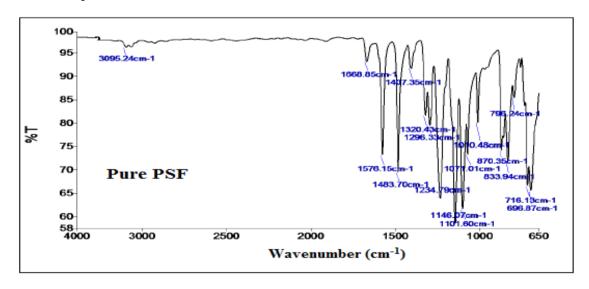


FIGURE 3. FT-IR Spectrum of pure Polysulfone (PSF)

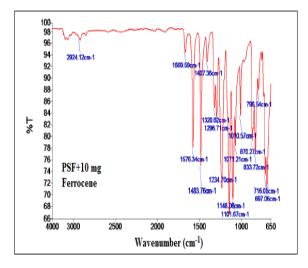
FT-IR spectrum of pure PSF exhibits specific characteristics peaks which can be widely distinguished into four regions, 600-1000 cm<sup>-1</sup>, 1100-1400 cm<sup>-1</sup>, 1500-1600 cm<sup>-1</sup> and 2900-3100 cm<sup>-1</sup>. The main bands of interest in the FT-IR spectrum

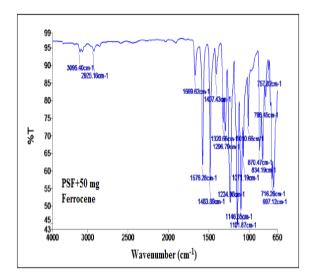
of pure PSF are 3095.24 cm<sup>-1</sup>, 1576.15 cm<sup>-1</sup>, 1296.33 cm<sup>-1</sup>, 1146.07 cm<sup>-1</sup>, 870 .35 cm<sup>-1</sup> and 796.24 cm<sup>-1</sup>. The peak corresponds to higher range of wave number 3095.24 cm<sup>-1</sup> is due to stretching of aromatic C-H bond present in PSF[21]. From



previous reported work it has been established that aromatic ring is retained in the polymers [14]. The band appears at 1576.15 cm<sup>-1</sup> and 1483.70cm<sup>-1</sup> is attributed due to stretching of C<sub>6</sub>H<sub>6</sub> ring. The asymmetric stretching vibration of aryl-ether-group C-O-C appears at 1296.33 cm<sup>-1</sup>. The vibrational band located at 1146.07 cm<sup>-1</sup> normally corresponds to symmetric stretching of sulfone group O=S=O.

The band located at 870.35 cm<sup>-1</sup> is due to C-H bond out of plane bending vibration [21]. The absorption band corresponding to the region from 696.87 cm<sup>-1</sup> to 796.24 cm<sup>-1</sup> indicates presence of C=C functional group in PSF [15].The FT-IR spectra of PSF doped with 10 mg, 50 mg and 100 mg of ferrocene are presented in figure 4,5 and 6 respectively.





**FIGURE 4.** FT-IR Spectrum of PSF+10 mg Ferrocene FIGURE 5. FT-IR Spectrum of PSF+50 mg Ferrocene

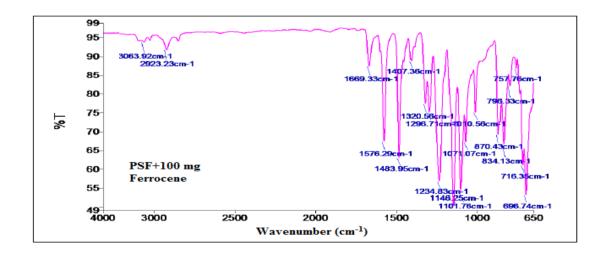


FIGURE 6. FT-IR Spectrum of PSF+100 mg Ferrocene

The FT-IR spectra of PSF sensitized with ferrocene indicates some shift in bands due to chemical interaction between chain of host polymer matrix

and molecules of low molecular weight dopant material. The band of pure PSF corresponding to 3095.24 cm<sup>-1</sup> is shifted to 2924.12 cm<sup>-1</sup>, 3095.40



cm<sup>-1</sup> and 3063.92 cm<sup>-1</sup> as doping concentration (10 mg, 50 mg and 100 mg) increases respectively. Similarly, the band 1576.15 cm<sup>-1</sup> of pure PSF is shifted to 1576.43 cm<sup>-1</sup>, 1576.28 cm<sup>-1</sup>, 1576.29 cm<sup>-1</sup> with increase in doping ratio. The band 1296.33 cm<sup>-1</sup> of pure PSF is also shifted to 1296.71 cm<sup>-1</sup>, 1296.79 cm<sup>-1</sup>, 1296.71 cm<sup>-1</sup>. In the same way all

specific important bands, which describes the structure of polysulfone shows some shifting due to doping. The band assignments of the FT-IR absorption bands for pure PSF and ferrocene doped PSF with their corresponding intensities have been presented in table 1.

**TABLE 1**. Different vibrational modes of various functional groups correspond to observed FT-IR characteristics of pure and ferrocene doped polysulfone

Assigning of Peaks	Pure PSF		PSF+10mg Ferrocene		PSF+10mg Ferrocene		PSF+10mg Ferrocene	
	Wavenumbe	%Intensit	Wavenumbe	%	Wavenumbe	%Intensit	Wavenumbe	%Intensit
	r cm <sup>-1</sup>	У	r cm <sup>-1</sup>	Intensit	r cm <sup>-1</sup>	У	r cm <sup>-1</sup>	У
				У				
Aromatic								
С-Н	3095.24	96.53	2924.12	96.25	3095.40	94.04	3063.92	93.94
stretching								
Stretching								
due to	1576.15	73.29	1576.34	72.10	1576.28	61.87	1576.29	61.60
C <sub>6</sub> H <sub>6</sub> ring								
Assymetri								
c stretch of	1296.33	79.57	1296.71	78.81	1296.79	77.41	1296.71	75.29
C=O band								
Symmetre								
stretch of	1146.07	58.54	1146.06	56.68	1146.35	51.76	1146.25	50.27
S=O band								
C-H band	870.35	74.24	870.27	73.25	870.47	65.86	870.43	64.38
C=C band	796.24	85.47	796.54	83.04	796.45	81.12	796.33	80.31

The broadening of bands from 550 cm<sup>-1</sup> to 850cm<sup>-1</sup> clearly apparent after doping the polysulfone with ferrocene may be corresponding to the vibration of C<sub>5</sub>H<sub>5</sub>-Fe-C<sub>5</sub>H<sub>5</sub> linkage of ferrocene material with PSF. Every absorption band of pure PSF shows slight shifting, which may be due to the linking of PSF with functional groups of ferrocene; however it is noticeable that mixing of ferrocene is not producing any drastic modification in the structure of pure PSF. Hence, we predict a good and suitable chemical interaction between pure PSF and ferrocene. The development of new absorption band at 1407 cm<sup>-1</sup> appears in doped samples illustrated the

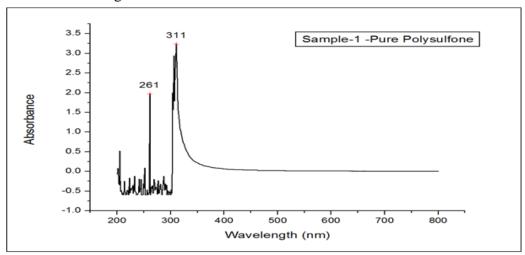
attribution of ferrocene in polysulfone. As per the FT-IR spectra study, it is also observed that the transmittance of all remarkable absorption peaks of

pure PSF decreases, as doping concentration increases. This is due to chemical bonding between PSF chains and ferrocene molecules. Hence we can understand that molecules of ferrocene is linking with chain of PSF and restricting the transmission of light. So, it is proposed that ferrocene is a suitable dopant for pure polysulfone and this kind of doping may enhance the characteristics of polysulfone.



Ultraviolet-Visible Spectroscopy (UV): To study the optical properties of polysulfone, the UV-Visible absorption spectrum is recorded. The UV-Visible spectroscopy is well established characterization technique to measure absorbance by the materials as a function of wavelength, when material is exposed in UV radiation [16]. For visible and ultra-violet spectrum, electronic excitation occurs in the range of 200-800 nm. The transitions in the range of 200-390 nm are in ultra-violet region and transitions

correspond to 390–780 nm are in the visible region. The UV spectrum of a material consists of a broad band of absorption centered near the wavelength of the major transitions. The estimation of highest absorbed wavelength by the material further led to calculations of energy associated with radiation, optical band gap ,type of electronic transitions, extinction coefficient etc. The UV-Visible spectra of pure polysulfone (PSF) is presented in figure 7.

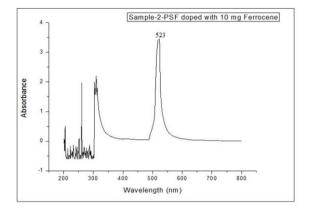


**FIGURE 7.** UV-Visible spectra of pure PSF

The optical absorption spectra of pure PSF are recorded in the wavelength region 200 nm to 800 nm. The spectrum of pure PSF demonstrated a sharp absorption peak at wavelength 311 nm which is on higher side of UV range (200-390 nm). This band at 311 nm wavelength attributed  $\pi \rightarrow \pi^*$  transition. This type of transition occurs in the unsaturated centers of the molecules. It is found mostly in the compounds containing double or triple bonds and also in aromatic polymers. The excitations of  $\pi$  electrons require smaller energy and hence

transition appears at longer wavelength. The band gap can be calculated by the formula  $E=hc/\lambda$ . The band gap of pure PSF is estimated as 3.99 eV. The sharp absorption band of pure PSF was found to shift towards higher wavelength region with increase in doping of ferrocene in polysulfone. This shifting of absorption peak of pure PSF for concentration of doping of ferrocene as 10 mg, 50 mg and 100 mg of is presented in figures 8, 9 and 10 respectively.





Sample-3-PSF doped with 50 mg Ferrocene

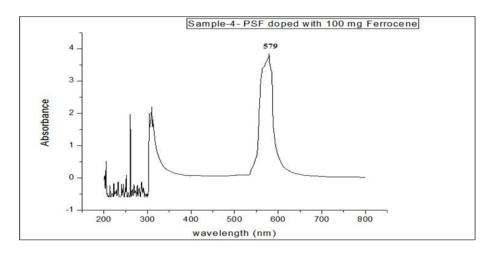
545

2200 300 400 500 600 700 800

Wavelength (nm)

**FIGURE 8.** UV- Visible spectra of PSF+10 mg Ferrocene

**FIGURE 9.** UV-Visible spectra of PSF+50 mg Ferrocene



**FIGURE 10.** UV-Visible spectra of PSF+100 mg Ferrocene

$$\frac{n^2 - 1}{n^2 + 2} = 1 - \sqrt{\frac{E_g}{20}}(1)$$

The sharp absorption bands for doped samples of concentration 10 mg, 50 mg and 100 mg are shifted to higher wavelength 523 nm, 545 nm and 579 nm respectively. It is observed that absorbance of doped samples increases with concentration. This effect can be explained by assuming that molecules of dopant material is establishing suitable linking with polymer matrix and restricting the transmission of light. This results in enhancement of absorbance. The band gap for doped samples has also been calculated and found that band gap decreases gradually concentration of doing increases. The refractive indices (n) of pure PSF and ferrocene doped samples calculated by using the undermentioned mathematical relation [17].

The determined band gap (E<sub>g</sub>) and refractive index (n) values of pure PSF and ferrocene doped samples have been presented in Table 2. It is observed from table 2 that value of band gap decreases while refractive index increases with increase in doping concentration. The enhancement of refractive index also indicates towards blocking of transmission of UV-Visible radiation and thus absorption increases as doped films become denser gradually. The estimation of band gap is essential parameter to study the enrichment in electrical properties of polysulfone.



**TABLE 2**. Absorbance onset wavelengths and optically determined bandgaps for the pure and ferrocene doped polysulfone

Polymer Samples	Absorption	Bandgap (eV)	Refractive Index
	onset(nm)		<b>(n)</b>
Pure PSF	311	3.99	2.15
PSF+10mg Ferrocene	523	2.37	2.61
PSF+50mg Ferrocene	545	2.27	2.61
PSF+100mg Ferrocene	579	2.14	2.71

**X-Ray Diffraction Spectroscopy (XRD):** The X-Ray Diffraction spectroscopic analysis (XRD) technique is a non-destructive method and reveals the detailed analysis of crystallographic structure, chemical composition and physical properties of material [18]. In the XRD pattern the Sharp peak represents crystalline region and diffused peaks exhibit amorphous regions of polymers. The XRD patterns for pure and doped polysulfone samples for

2θ parameter are obtained in the range of  $0^0$  to  $90^0$ . The crystallite size was calculated using Scherrer's formula (P=K $\lambda$ /βcosθ). The Full Width of Half Maximum (FWHM) and distance between the planes (d-spacing) of internal structure of polysulfone is also estimated by curve fitting technique. The XRD pattern of pure PSF and PSF doped with 10 mg, 50 mg and 100 mg of ferrocene have been presented in figures 11,12,13 and 14 respectively.

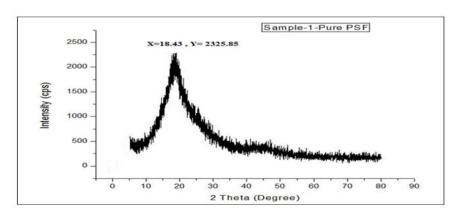
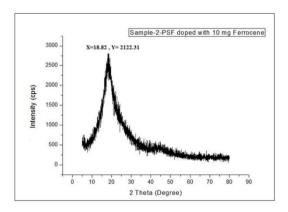


FIGURE 11. XRD pattern of pure PSF



**FIGURE 12.** XRD pattern of PSF+10 mg Ferrocene Ferrocene

**FIGURE 13.** XRD pattern of PSF+10 mg



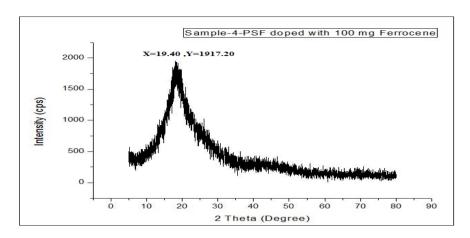


FIGURE 14. XRD pattern of PSF+100 mg Ferrocene

The XRD pattern of pure PSF is a combination of both sharp and diffused peaks. Polysulfone is a amorphous polymer. The sharp peak of pure PSF is obtained at 18.43° and rest of the peaks are diffused peaks which justify the amorphous structure of polysulfone. The Intensity corresponding to one sharp peak is recorded 2325.85 cps. The FWHM for pure PSF has been found as 11.79°. The d-spacing and crystallite size have been calculated as 0.48 nm and 0.71 nm respectively. The parameters FWHM, d-spacing and crystallite size are very essential parameters to understand the internal chemical structure of material. The XRD patterns of ferrocene

doped samples indicates slight shift in the location of sharp peak of pure PSF. The location of sharp peak has been recorded at  $18.82^{\circ}$ ,  $19.01^{\circ}$  and at  $19.40^{\circ}$ for doping concentration as 10 mg, 50 mg and 100 ferrocene in **PSF** respectively. The mg corrsponding intensities of theses sharp band have recorded as 2122.31cps, 1944.51 cps and 1917.20 with these specific cps doping concentration. The essential XRD parameters of pure and sensitized samples have been presented in table3.

**TABLE 3**.XRD parameters for pure and ferrocene doped polysulfone

Polymer Samples	Position(2θ)	d-Spacing	FWHM(β)	Intensity	Average Crystallite
	(Degree)	(nm)	(Degree)	(cps)	size(P) (nm)
Pure PSF	18.43	0.48	11.79	2325.85	0.71
PSF+10mg	18.82	0.47	11.88	2122.31	0.71
Ferrocene					
PSF+50mg	19.01	0.47	12.51	1944.51	0.67
Ferrocene					
PSF+100mg	19.40	0.46	12.81	1917.20	0.66
Ferrocene					

It is reflected from the analysis of XRD parameters for doped samples that position of sharp peak of pure PSF is shifted towards highier angle. This shfting is due to the linking of atoms of dopant with host polymeric chain .This action increases crystallization of PSF and produces minimization of



crystal defects. The full width of half maximum is found as 11.79<sup>0</sup> for pure PSF. The peak broadning is clearly apparent as the full width of half maximmum (FWHM) increases to 11.88°,12.51° and 12.81<sup>0</sup> gradually for 10 mg, 50 mg and 100 mg ferrocene doped samples. It is noticeable from table 3 that average crystallite size decreases from 0.71 nm to 0.67 nm and 0.66 nm respectively with the increase in degree of senstization. It is reported in earlier studies that smaller crystals produce broader XRD peaks. The peak broadning with decreasing crysallite size confirms the reduction in particle size as content of ferrocene increases in polysulfone. Thus the incorporation of ferrocene does not produce any new additional sharp peak but produced modification by reducing crystallite size in the strcture of polusulfone reveals successful doping of ferrocene in the lattics of pure PSF. From table 3, it is observed that strucural modifications like reduction in interplaner distance (d) and average crystallite size (P) occurs in pure PSF due the doping of ferrocene. This causes, drastic transformation in overall properties of the PSF.

## **CONCLUSION**

PSF and PSF-ferrocene composite thin films with doping concentration of ferrocene as 10 mg, 50 mg and 100 mg in 4 gm of PSF were produced by isothermal immersion technique .The thickness of these pure and doped foil films was observed as ranging from 0.50 to 0.53 microns. The micro analysis about chemical composition and complete characterization of these samples was carried out by FT-IR and **UV-Visible** XRD, spectroscopic techniques. Based on mathematical calculations of all essential parameters of spectroscopic techniques and analysis of spectrum, it was observed in this study that incorporation of ferrocene within PSF matrix shows good compatibility. The sensitization of PSF with ferrocene produces considerable alteration in the characteristics of PSF.FT-IR spectrum analysis exhibited that all remarkable peaks corresponding to pure PSF, were also

obtained for ferrocene doped PSF, but with slight shifting and decrease in the intensity, with increase in the doping concentration. The broadening and lowering in intensities of peaks with doping concentration established a good chemical interaction between PSF and ferrocene. It is proposed that Charge Transfer Complexes (CTC) established between PSF and ferrocene due to the exchange of charge between donor and acceptor molecules. The process of CTC formation between two materials occurs due to the transfer of electron from electronegative material ferrocene to polymer polysulfone. The ferrocene has one C<sub>5</sub>H<sub>5</sub><sup>-2</sup> group with unshared pair of electron, which is expected to be taking part in the CTC formation with PSF. The development of a new peak only in doped samples at around 1407 cm<sup>-1</sup> may be a significant characteristic caused by ferrocene to property of PSF. The analysis of optical properties of PSF was carried out through UV-Visible spectroscopy over a broad range of wavelength from 200 nm to 800 nm. Under this testing ,the absorbance of pure and ferrocene sensitized PSF was measured. The absorption of higher wavelength was obtained, with increase in doping. The pure PSF absorbs UV wavelength (200-390 nm), while ferrocene doped PSF absorbs visible wavelength (400-800 nm). It was observed by the UV spectrum analysis that incorporation of ferrocene in PSF, established suitable chemical interaction between ferrocene and PSF. Ferrocene molecules were linking appropriately with polymer bands and increase the density of PSF. The refractive index of all samples was calculated and found to be increasing with increase in doping concentration. This indicates that PSF become denser as content of ferrocene increases. As density of material increases the absorbance also increases. It was also estimated that band gap of doped samples gradually decreases as doping ratio increases. The lowering of band gap causes a important characteristic enhancement in electrical of conductivity of PSF. The XRD analysis was carried out, to study the internal chemical structures of



materials and alteration in their structure due to mutual chemical interaction between PSF and ferrocene. It is observed by the calculations of XRD parameters that crystallite size of PSF decreases with increase in ferrocene doping concentration. This action reduces the molecular size of pure PSF up to micro and nano range, due to which PSF will be a alternate material in some remarkable electronic devices, which require nanosized molecular structure of the material. The attempt of doping of ferrocene in PSF has not been tried by any of the researcher, so far in the study. Therefore, it is expected that the present study involving the use of ferrocene in PSF will bring some new dimensions in the polymer study. It has been already reported in earlier studies that polymers exhibit good dielectric and electrical properties and hence applicable in various electronic devices. It is proposed through this research work that ferrocene doped PSF will exhibit best possible dielectric behavior efficient electrical and conduction, due to the formation of charge transfer complexes (CTC) between ferrocene and PSF. The various solid state devices designed with this new composite material (PSF with Ferrocene) will definitely show considerable efficiency at low cost.

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