



## Complex Optical Study of Chemically Synthesized Polypyrrole

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Available online at: [www.isca.in](http://www.isca.in), [www.isca.me](http://www.isca.me)

Received 22<sup>nd</sup> March 2016, revised 30<sup>th</sup> March 2016, accepted 15<sup>th</sup> April 2016

### Abstract

*In the present work, different complex optical parameters were computed for chemically synthesized polypyrrole (PPy). The absorbance, extinction coefficient, refractive index, optical conductivity, real and imaginary dielectric constants were considered as complex optical parameters. The average polymer chain separation for as-synthesized PPy computed using X-Ray Diffraction (XRD) technique. Simple approach that is ultraviolet-visible spectroscopy was employed to investigate complex optical parameters. The obtained results are found compatible with recent reports in literature and found suitable for terahertz technology application.*

**Keywords:** Complex Optical Parameters, Polypyrrole, Terahertz device.

### Introduction

Conducting polymers are very important class of materials science. The optical and thermal properties of conducting polymers are very wonderful and have very interesting applications. Al-Mashat et al synthesized polypyrrole nanofibers by template-free chemical route for hydrogen gas sensing at room temperature<sup>1</sup>.

The optical and electrical properties of chemically synthesized thin films of polyaniline and polypyrrole were investigated by Abdulla et al. The electronic spectrum frequencies were used to determine basis using Density Functional Theory. After summarizing the results, it is clear that polyaniline shows satisfactory results for optical absorption<sup>2</sup>.

The potentiostatic electrodeposition technique was adopted by Thombare et al for synthesis of polypyrrole thin films. In this process, electrodeposition voltage maintained at +0.7 V between reference and calomel electrode. The effect of different electrolytes on complex optical parameters was investigated<sup>3</sup>.

The pure and doped form of polypyrrole was synthesized using different protonic acids (HCl and H<sub>3</sub>PO<sub>4</sub>) by Saxena et al. In this synthesis, NaOH was used as reducing agent in aqueous HCl medium whereas ammonium persulphate as an oxidizing agent<sup>4</sup>.

In light of above discussion, we planned to explore the complex optical properties of chemically synthesized PPy. In complex optical parameters, some crucial parameters like absorbance, extinction coefficient, refractive index, optical conductivity, real and imaginary dielectric constant were investigated.

### Methodology

AR chemicals were used for the synthesis of PPy without further purification. The chemical oxidative polymerization route was adopted for the synthesis of PPy. Pyrrole monomer and TiCl<sub>4</sub> were used as starting chemicals. The wt. % stoichiometry was employed for the preparation of sample by using monomer and oxidant wt.% ratio as 75:25.

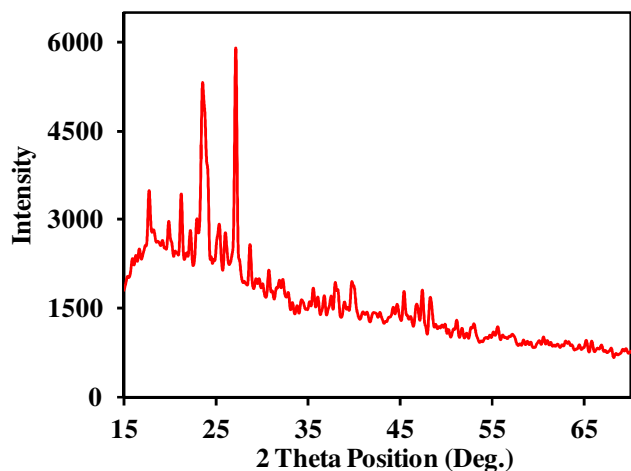
The polymerization reaction was carried out at room temperature (297 K). The as-obtained polymer was several time wash using distilled water. The as-prepared materials were characterized using X-ray diffractometer (XRD) (Rigaku Miniflex-II, X-ray diffractometer, Japan). The surface topography of as-synthesized sample was analyzed with the help of scanning electron microscope (SEM) (JEOL JSM-7500F, Japan). The ultraviolet-visible spectroscopy data recorded using Agilent UV-VIS spectrometer Carry-60.

### Results and Discussion

The XRD pattern of chemically synthesized PPy is shown in Figure-1. The XRD pattern of PPy comprises some sharp peaks and noise. It indicates that PPy is in semi-crystalline state. Generally, chemical oxidative polymerization of pyrrole monomer leads to amorphous state, but strong oxidation potential of TiCl<sub>4</sub> used as oxidant, improve degree of crystallization. Average chain separation (ACS) values of PPy sample is determined using the relation<sup>5</sup>.

$$ACS = \frac{5\lambda}{8\sin\theta}$$

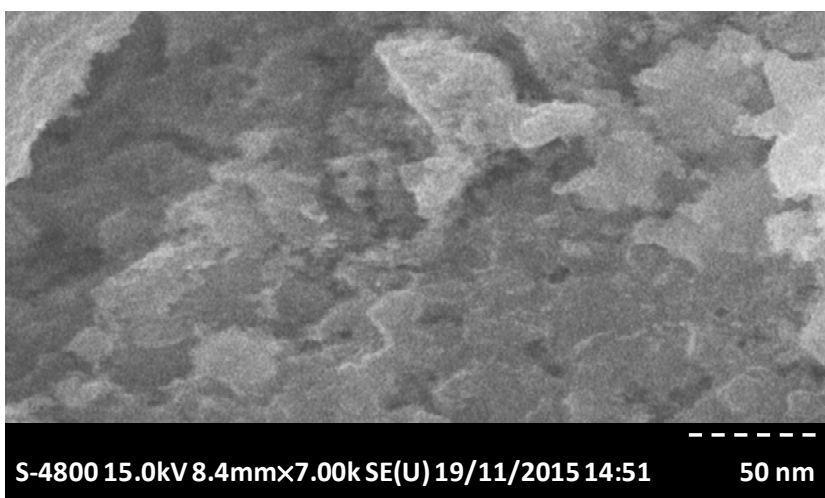
where: R is the polymer chain separation in Å,  $\lambda$  is the X-ray wavelength (1.541 Å) and  $\theta$  is the Bragg's angle having the high intensity. The ACS value was found to be 1.054 Å.



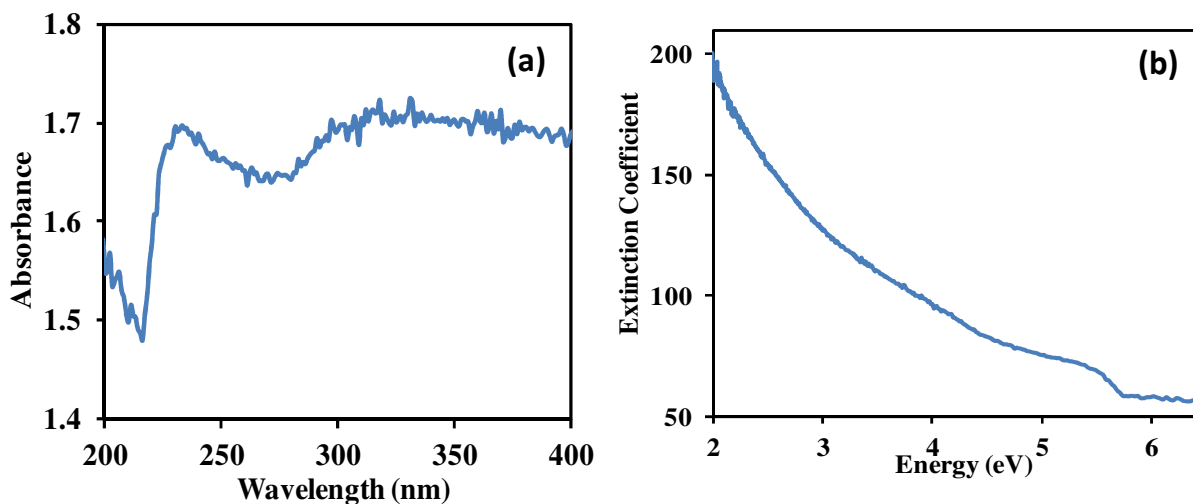
**Figure-1**  
XRD pattern of chemically synthesized PPy

Figure-2 shows the SEM image of PPy sample. The micrograph shows that final product is in semi-crystallized form. This highly ordering of PPy sample attributed to use of  $\text{TiCl}_4$ . The good degree of polymerization concluded from XRD analysis is supported by SEM analysis.

Figure-3a depicts the UV-VIS spectra of chemically synthesized PPy sample. The spectra shows that sample shows intense absorption hike around 221 nm. After 250-400 nm, absorption is nearly linear. Figure-3b represents the variation of extinction coefficient as a function of photon energy of PPy sample. The value of extinction coefficient decreases in nearly exponential manner from 2-5.8 eV. This indicates that sample traps longer wavelength effectively than lower wavelength<sup>6</sup>.



**Figure-2**  
SEM image of chemically synthesized PPy



**Figure-3**  
(a) UV-VIS spectra and (b) Extinction coefficient of chemically synthesized PPy

Figure 4 (a) and 4 (b) depicts the variation of refractive index as a function of wavelength and optical conductivity as a function of photon energy, respectively. The results of refractive index are in congruence with absorption analysis of sample. The values of refractive index increase sharply around 221 nm and settle near to unity between 290-590 nm. Similarly, optical conductivity value found nearly constant between 3-5 eV.

Figure-5 shows the variation of real and imaginary dielectric constant. The real dielectric constant is depends on refractive index. It is very well known behavior that, the electromagnetic

radiations slows down in denser medium. In our case, medium is polymeric material which obeys Functional Density Theory. It is observed that both curve decreases exponentially with photon energy up to 5.5 eV. In between 5.5-6.5 eV, real and imaginary dielectric constant curves remains almost constant. Imaginary dielectric constant indicates the degree of interaction between an electric field and dipole present in medium. In our case, imaginary dielectric constant was found to be higher for lower energy photons. But, it gradually decreases with increasing photon energy and settle down beyond 5.5 eV.<sup>7,8</sup>

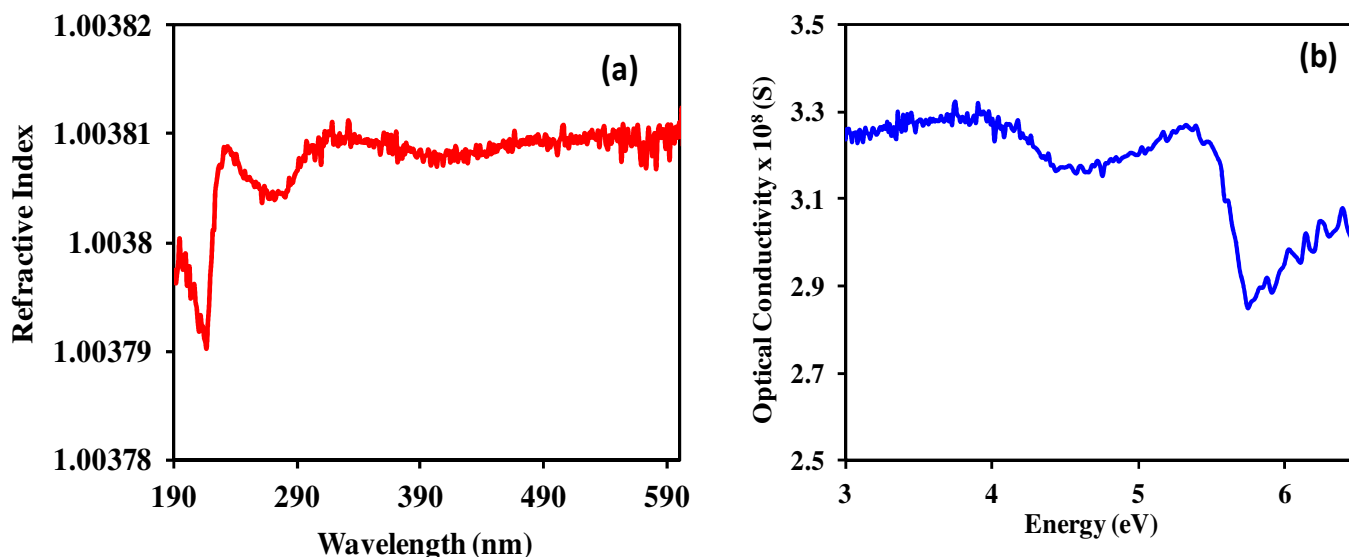


Figure-4  
(a) Refractive index spectra and (b) Optical conductivity spectra of chemically synthesized PPy

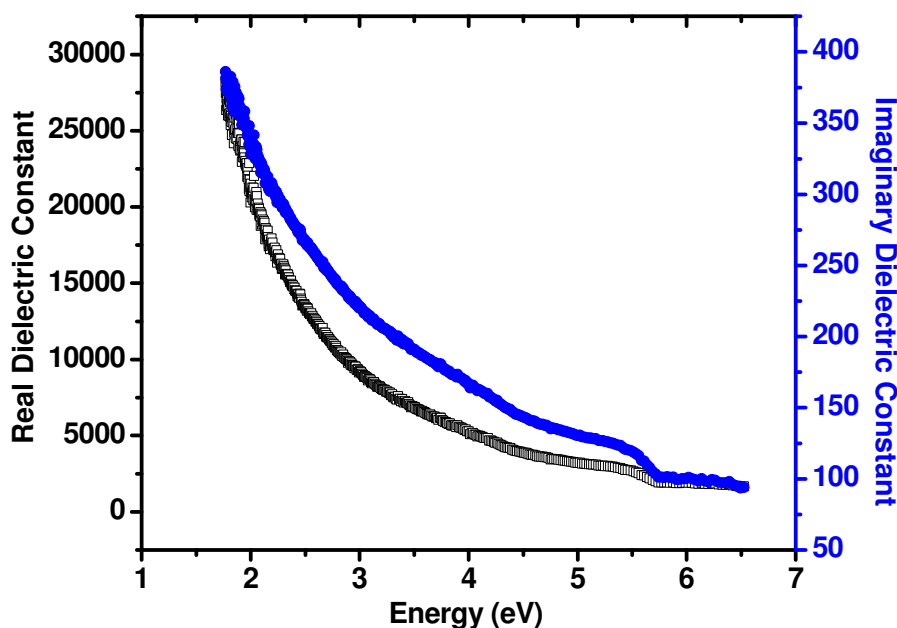


Figure-5  
Plot of real and imaginary dielectric constant as a function of photon energy

## Conclusion

In our present work, we conclude that PPy was successfully synthesized and used to analyze complex optical parameters. The ACS value was found to be 1.054 Å, determined using XRD analysis. The measurement of extinction coefficient of sample shows that sample strongly traps longer wavelengths. Moreover, sample has considerable properties of real and imaginary dielectric constant.

## Acknowledgement

The most of the work presented in this article was carried out at Department of Physics, Sant Gadge Baba Amravati University, Amravati. The authors are gratified to Head, Department of Physics Sant Gadge Baba Amravati University, Amravati for providing necessary facilities.

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