Quest Journals
Journal of Electronics and Communication Engineering Research
Volume 6 ~ Issue 2 (2020) pp: 29-33
ISSN(Online) : 2321-5941
www.questjournals.org

Research Paper

Estimation of the refractive index and dielectric constants of tin phthalocyanine oxide thin films from its optical studies

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ABSTRACT: *Tin phthalocyanine oxide (SnPcO) thin films were prepared at room temperature by vacuum sublimation under a pressure of* 10^{-5}*Torr. The optical absorption and reflectance spectra of SnPcO thin films were recorded over the wavelength range 300-900 nm using the Shimadzu 160 A spectrophotometer. The absorption coefficient α and extinction coefficient k were calculated from the absorption spectra. Using α and k, the refractive index n and the real and imaginary parts of the dilectric constant* ϵ_1 *and* ϵ_2*were determined. Variation of n, k,*ϵ_1 *and* ϵ_2 *with the photon energy for tin phthalocyanine oxide thin films were plotted.*

KEYWORDS*: Organic semiconductor, phthalocyanine, thin film, band gap, absorption coefficient, extinction coefficient, refractive index*

Received 16November, 2020; Accepted 05 December, 2020
Published with open access at ***www.questjournals.org***

I. INTRODUCTION

Thin films find great use in a variety of active and passive microminiaturised components and devices, solar cells, radiation sources and detectors, magnetic memory devices, sensors and high density memory systems for computers because of their compactness, better performance and reliability, low cost of production and low package weight.

Organic semiconductors are of great interest in many thin film applications because of their ability to modify their molecular structure and hence their electrical and optical properties. Among the organic semiconductors, phthalocyanines are the most extensively studied materials because of their stability against thermal and chemical decomposition and intense absorption in the visible spectrum. Due to their intense colouring properties, they are used as pigments in many industrial paints and in inks for colour laser printing and they are also used as the data storage layer of many CDs [1]. Organic field effect transistors based on single crystalline copper phthalocyanine (CuPc) ribbons [2] and organic solar cells with a nanostructuredCuPc layer[3] are also reported. The phthalocyanines are structurally similar to naturally occurring porphyrins such as haemoglobin, chlorophyll and vitamin B12. The role of the metal atom phthalocyanine molecule is of interest in several fields where phthalocyanines find application such as for photovoltaic energy conversion [4,5,6] and catalysts in electrochemical reaction process [7]. Davidson has shown that the optical properties of phthalocyaninesare sensitive to substitution of the central metal atom [8]. For probing the band structure in semiconductors , one of the most direct methods is the optical absorption studies. We can determine the energy gap of the material by knowing the frequency dependence of the absorption process. Rapid drop in the absorption coefficient on the high energy side of the absorption band leads to a band edge which can be analysed to get the band gap of the material.

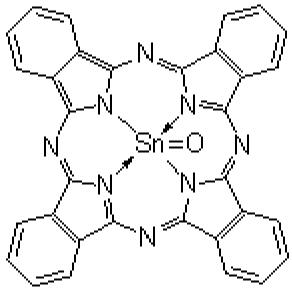

Figure1: The molecular structure of SnPcO

The interest in tetravalent SnPcO molecule is motivated by its peculiar nonplanar shape. It is a less investigated material also. The central metal atom of SnPcO stands out of the macrocycle. This gives rise to directional anisotropy and selectivity in the absorption geometry as well as in the intermolecular stacking. In the present work the refractive index and dielectric constants of tin phthalocyanine oxide thin films are determined from its absorption coefficient and extinction coefficient.

II. EXPERIMENT

Tin phathalocyanine oxide powder procured from Aldrich, USA is used as the source material for the preparation of the thin films. Thin films are deposited onto thoroughly cleaned glass substrates at room temperature using a Hind Hivac 12 A4 coating unit at a base pressure of 10^{-5}Torr. The films are prepared by resistive heating of the powder from a molybdenum boat and the evaporation rate is controlled within the range 10-12 nm /min by regulating the current. A variable voltage transformer provided in the circuitry facilitates the precise control of current through the molybdenum boat. Thickness of the film is determined by Tolansky's multiple beam interference technique [9]. UV-VIS absorption and reflection spectra over the wavelength range 300-900 nm are recorded using the Shimadzu 160 A spectrophotometer. The absorption and reflection spectra are analysed to evaluate the refractive index n , the extinction coefficient k and real and imaginary parts of dielectric constants $\epsilon_1$andϵ_2

III. RESULTS AND DISCUSSION

The absorption spectrumofSnPcO thin film is recorded in the wavelength range 300-900nm. The UV-VIS spectrum obtained for metal phthalocyanines originates from the molecular orbitals within the aromatic 18 π electron system and from overlapping orbitals on the central metal atom[10]. The distinct characterized absorption bands are the fundamental absorption at high energies (B-band) and the exciton absorption at low energies (Q-band). They are generally interpreted in terms of $\pi - \pi^*$ excitation between bonding and antibonding molecular orbitals[11].Figure 2 shows the absorption spectrum of SnPcO thin film of thickness 294 nm deposited at room temperature. Absorption peaks are observed at around 377 nm and 744 nm. The peaks, at high energy region (377 nm) and at low energy region (744nm) are taken as the B-band and the Q-band peaks respectively. The absorption at the lower energy side is ascribed as exciton absorption and has been confirmed for many other phthalocyanines [12,13].

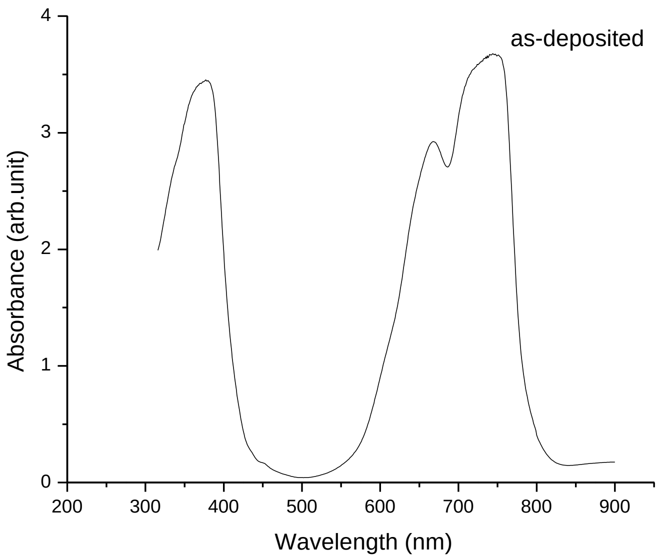

Figure2: Absorption spectrum of SnPcO thin film of thickness 294 nm deposited at room temperature

The absorption coefficient α is calculated using equation

α= 2.303 A/t (1)

where A is the absorbance of the film and t is its thickness. The electronic transitions between the valence and the conduction bands can be direct or indirect. In both cases it can be allowed as permitted by the transition probability (p) or forbidden when no such probability exists. The transition probability is related to α by the relation

α =A $(h\nu-E_g)^P$ (2)

Where$E_g$is the energy gap and p has discrete values like 1/2, 3/2, 2 , 3 or more depending on whether the transition is direct or indirect and allowed or forbidden [14]. In the direct and allowed cases the index p=1/2 whereas for the direct but forbidden cases it is 3/2. But for the indirect and allowed cases n=2 and for the indirect forbidden cases it will be 3 or more. Thus a linear graph when α^2 is drawn against hν, will suggest a direct allowed transition, whereas a linear one with $\alpha^{1/2}$ against hν indicates an indirect allowed transition. The magnitude of p can also be estimated from the slope of the graph of log αversus log hν and hence can suggest the type of transition. By extrapolating the linear portion of the graph to α= 0, one can obtain the band gap of a material.The plot of α^2 versus hν for SnPcO thin film deposited at room temperature is given in figure 3. The fundamental band gap is found to be 3.07eV for SnPcO thin film.

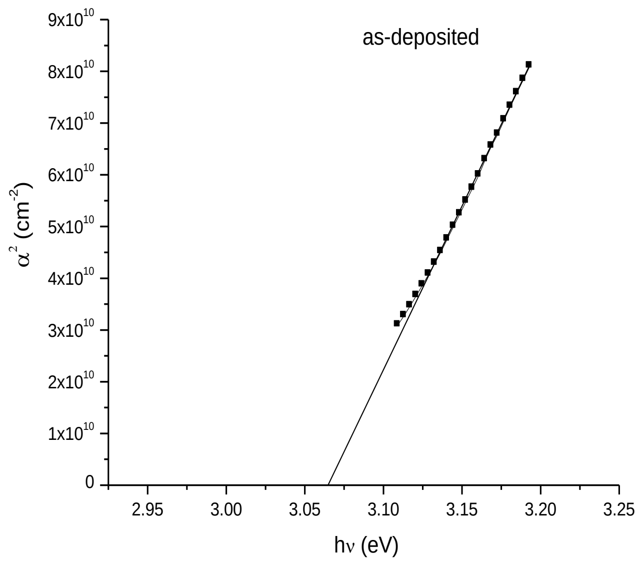

Figure 3.α^2 versus hν for SnPcO thin film of thickness 294 nm deposited at room temperature

The reflectance spectrum of SnPcO thin film deposited at room temperature is recorded and is given in Figure 4.

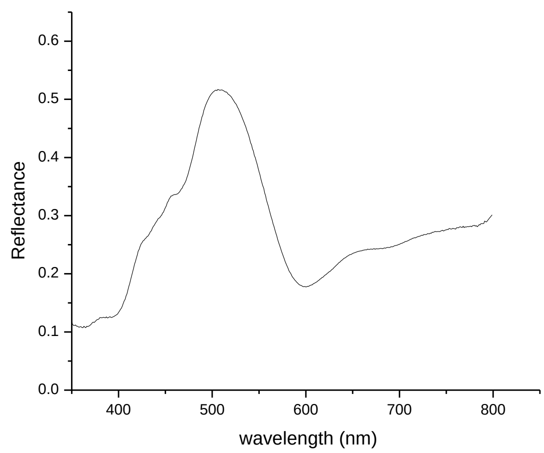

Figure4: The reflectance spectrum of SnPcO thin film deposited at room temperature

The main feature of the reflection spectrum is the sharp rise in reflectivity at about 500 nm. The optical properties of any material are characterized by two parameters k and n. The extinction coefficient k and the refractive index n are calculated using equations 3 and 4.

$$k = \frac{\alpha\lambda}{4\pi} \quad (3)$$

The reflectivity of an absorbing medium of indices n and k in air for normal incidence is given by [15]

$$R = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2} \quad (4)$$

Figure 5 shows the variation of refractive index n and extinction coefficient k with photon energy for SnPcO thin film.

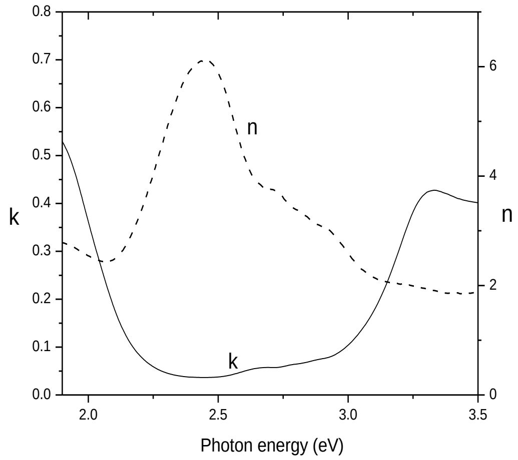

Figure5: Variation in refractive index n and extinction coefficient k as a function of photon energy for SnPcO thin film deposited at room temperature

The refractive index has a maximum value of 6.10 at 2.44 eV for the film of thickness 294 nm. Similar result is reported by Senthilarasu*et al* [16] for zinc phthalocyanine thin films. The refractive index and the extinction coefficient are used for the calculation of the real and imaginary parts of the dielectric constant. The real and imaginary parts of the dielectric constant ε_1 and ε_2 are calculated using the expressions 5 and 6[17].

$\varepsilon_1 = n^2 - k^2$ (5)

$\varepsilon_2 = 2nk$ (6)

The variation of ε_1 and ε_2 with photon energy for SnPcO thin film is shown in figure 6.

The real part ε_1 is related to dispersion, while the imaginary part ε_2 provides a measure of the dissipation rate of the wave in the material. The real part ε_1 showed maximum value at 2.44 eV for as-deposited SnPcO thin film. A similar behaviour has been observed for chloroaluminiumphthalocyanine thin films[15]. The scanning electron microscope (SEM) image of SnPcO thin film is taken for the investigation of surface morphology and microstructural feature and is shown in figure 7.

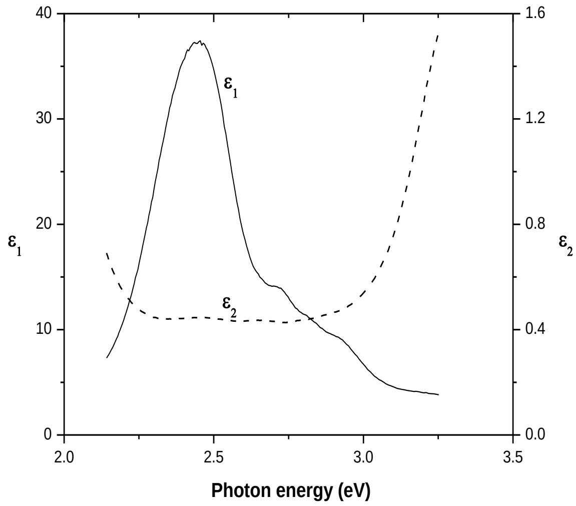

Figure 6: Plots of ε_1 and ε_2 versus photon energy for SnPcO thin film deposited at room temperature

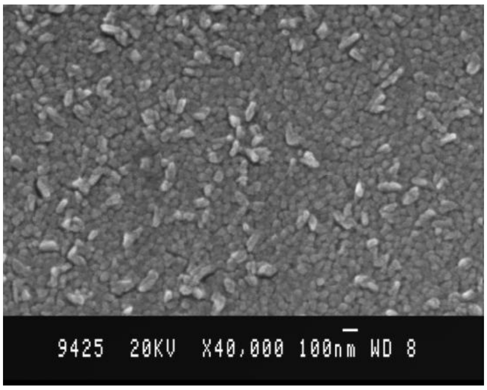

Figure7. SEM image ofSnPcO thin film

From the SEM planar view, it is clear that the film is made of homogeneous small crystal grains with grain size in the range 40 – 100 nm.

IV. CONCLUSION

Absorption spectrum of tinphthalocyanine oxide thin film has showed an enhanced broad optical window with lower linear absorption at about 500 nm. Tin phthalocyanine oxide film absorbs light on either side of blue-green region and can be used as photoconductor materials and colour filters.The optical band gap for tin phthalocyanine oxide thin film is determined as 3.07 eV. The spectral distribution of absorbance and reflectance measured at normal incidence facilitates the determination of the optical constants. The performance of the optical devices strongly depends on the wavelength dependence of the optical constants of their layers. Thin film material coatings on various substrates provide important functionalities for the micro fabrication industry and refractive index, extinction coefficient and thickness of these films must be measured and controlled to allow for repeatable manufacturing. SEM analysis reveals the uniform distribution of the grains over the substrate.

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Susan Mathew.“ Estimation of the refractive index and dielectric constants of tin phthalocyanine oxide thin films from its optical studies." *Quest Journals Journal of Electronics and communication Engineering Research,* Vol. 06, No. 02, 2020, Pp. 29-33.