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Structural, Optical and Electrical Characterization of Boron Subphthalocyanine Chloride Thin Films for Photovoltaic Applications

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Abstract: In the present work thin films of Boron Subphthalocyanine Chloride (sub pc) have been prepared by thermal deposition technique. The prepared films have been structurally characterized by X-ray diffraction (XRD), atomic force microscopy (AFM) and field emission scanning electron microscopic (FESEM) studies. The optical characterization of the film has been done by UV-Vis absorption spectrophotometry and by spectroscopic ellipsometric technique. The admittance spectroscopy of the film was done over five orders of frequency range. The carrier mobility through the films has been extracted by differential susceptibility method. Further,AC and DC conductivity of the sub pc film along with key dielectric parameters are also being reported. The Transport mechanism of carriers has been found to be hopping in nature.

Keywords: Boron Subphthalocyanine Chloride, Dielectric studies, Admittance Spectroscopy

I. INTRODUCTION

The field of photovoltaic cells using organic dyes has seen significant growth since the pioneer work done by W.Tang [1]. Among all the organic materials being explored for photovoltaic applications, metal phthalocyanines have exhibited promising results. This group of dyes consists of a central metal atom forming two covalent and two coordinate bonds with four nitrogen atoms linking four diiminoisoindoline groups. With the exception of Boron which has relatively smaller size, all metal phthalocyanines form a tetrameric structure. However, Boron, owing to its smaller size, can accommodate only three diiminoisoindoline groups and forms a trimeric analogue of its bulky counterparts. The unique bowl like structure (Figure 1) along with 14 pi conjugated electron system has attracted the attention of photovoltaic community [2]. A number of attempts have been reported using sub pc as active layer in the donor-acceptor geometry of hetro-junction solar cells. R. Pandey et al. has reported highest efficiency of 4.2% for graded sub pc/Fullerene (C60) cells. Some other attempts include work by H. Gommans et al. reporting an efficiency of 3.96%. Citing the potential application of the material, in the present work we are reporting complete structural, optical and electrical characterization of sub pc thin films [3-5].

II. EXPERIMENTAL TECHNIQUES

Sub pc procured from Sigma Aldrich company in powder form was used as such without any further purification. Thin films of sub pc were deposited on chemically and ultrasonically cleaned glass substrates by thermal evaporation using Hind High Vacuum coating unit under a residual air pressure less than 10-5 mbar. The Aluminum electrodes were deposited by shadow masking technique. The film thickness was monitored using quartz monitor during deposition and was

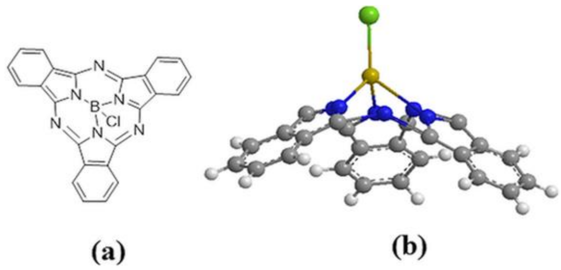


Figure 1: Chemical and spatial structure of sub pc

later confirmed by ellipsometeric studies using SE800 SENTECH ellipsometer and was found to be 50nm. The x-ray diffraction (XRD) studies were done using Kα line of Cu having wavelength 1.54 Å using Bruker Diffractometer in the range 100-800. The surface morphology of the deposited films was investigated by atomic force microscope (Nanosurf Easy Scan 2) and by Supra field emission scanning electron microscope. UV-Vis spectra were recorded with SHIMADZU, UV-VIS-NIR 3600 spectrometer in the wavelength region 200 nm to 1100 nm. The electrical measurements of the films were performed by admittance spectroscopy technique using Hioki 3522 LCR meter. All the electrical measurements were carried out under different bias conditions.

III. RESULTS AND DISCUSSION

X ray diffraction study of the film was performed (Figure 2) and was found to be amorphous as reported earlier in other independent studies[6, 7]. The FESEM image (Figure 3a) of the film show a uniform growth, with grain size of about 200 nm. A similar morphology was seen in the AFM image of the film (Figure 3b). The rms roughness of the sub pc film was found to be 3.8nm.

Figure 4(a and b) show the spectroscopic variation of the ellipsometric angles psi and delta for the sub pc film at an angle of incidence 700. The data was fitted using Lorentz oscillator model and the real and imaginary parts of the complex refractive index were extracted (Figure 5 a, b). The Uv-Vis analysis of the sub pc film show a strong absorption band around 590 nm (Q band) with a shoulder on the blue side, characteristic of the phthalocyanine family, along with B soret band in the UV region at 300 nm[2, 8]. The results obtained from UV-Vis studies and from ellipsometric studies are found to be in consonance with each other.

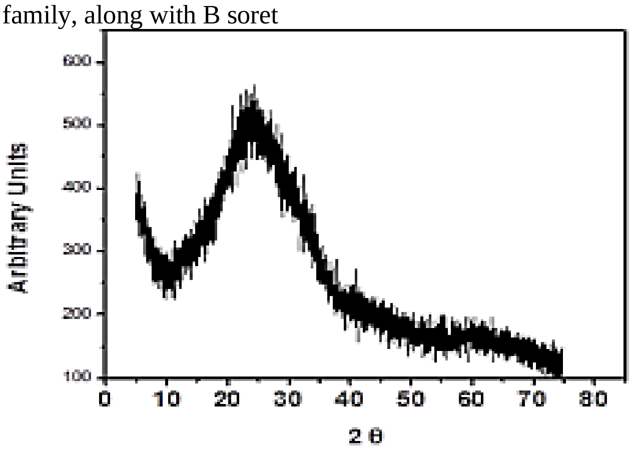
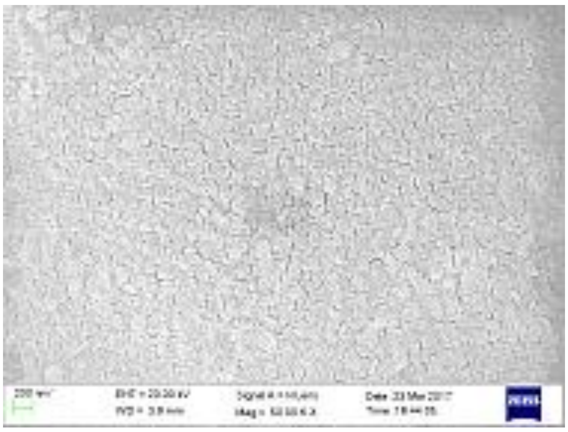
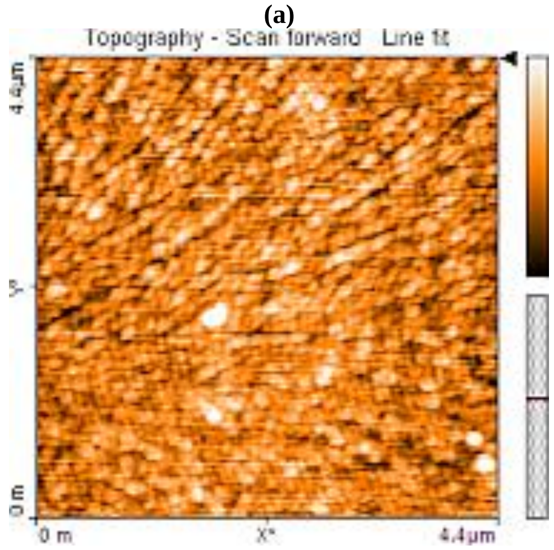


Figure 2: X ray diffraction spectrum of sub pc film

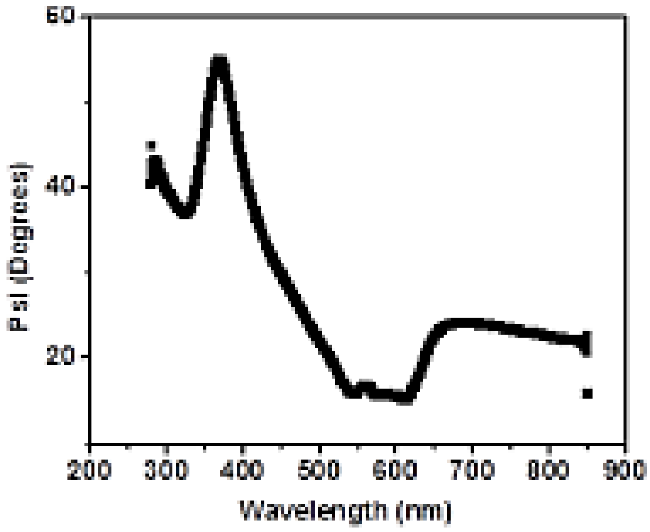


(a)

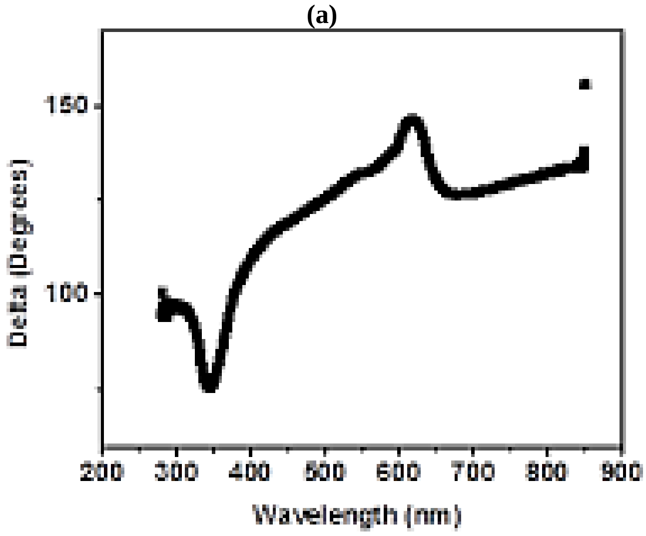


(b)

Figure 3: (a) FESEM (b)AFM image of sub pc film showing uniform growth



(a)



(b)

Figure 4: Variation of ellipsometric angles (a) Psi and (b) Delta with wavelength

The device with Al/sub pc/Al structure was electrically characterized over wide frequency range. Figure 6 represents variation of film capacitance with frequency of the external bias supply. The Capacitance of the films decreases uniformly and attains a constant value at high frequencies. This behavior of the organic dielectrics can be explained by Goswami and Goswami equivalent circuit model[9-12]. As per the Goswami equivalent circuit model, the total capacity consists of two components, frequency independent geometric capacity

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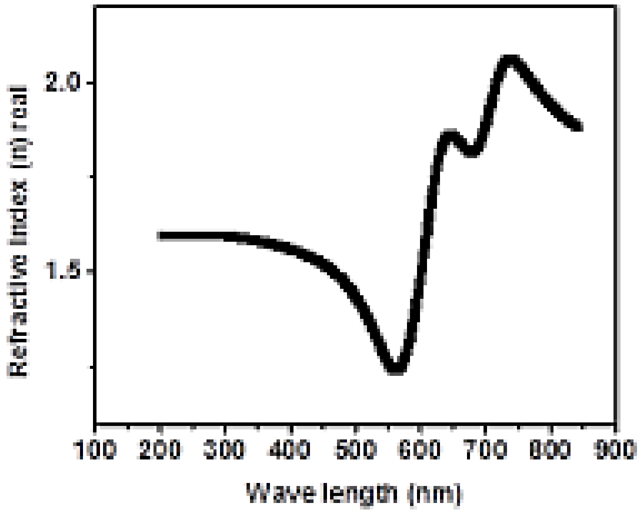
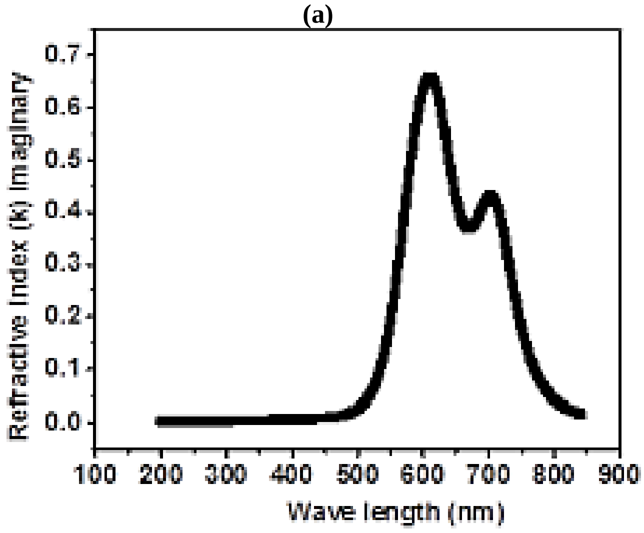
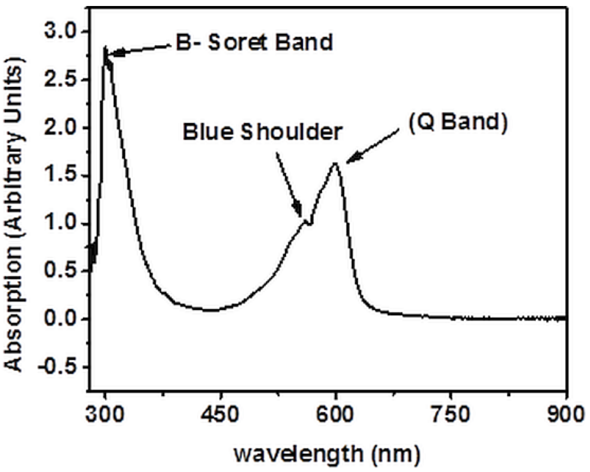


(a)



(b)

Figure 5: Spectroscopic variation of (a) real and (b) imaginary parts of refractive index



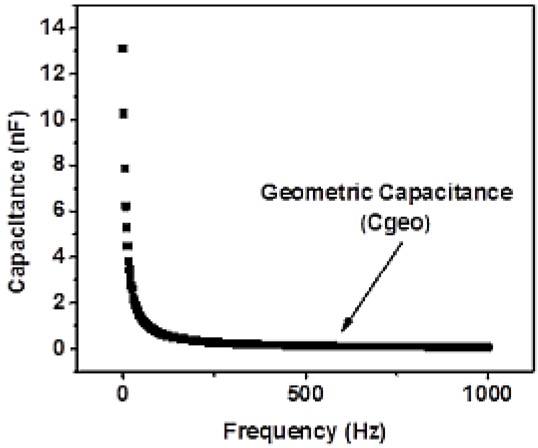


Figure 6: Spectroscopic variation of capacitance of sub pc film

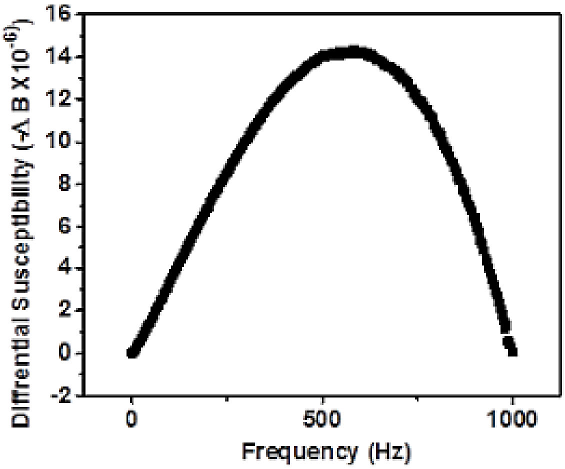


Figure 7: Spectroscopic variation of negative differential

Susceptibility of sub pc film and another part which varies with frequency. The contribution of the frequency dependent component goes on decreasing at high frequency range as charge carriers are unable to follow the fast varying AC bias. The asymptotic value of the capacitance curve represents the geometric capacitance (Cgeo). The carrier mobility was extracted from the differential susceptibility (-ΔB) curve (Figure 6) and was found to be $2.6 \times 10^{-8} cm^2V^{-1}s^{-1}$. The charge carrier concentration was determined from the slope of $1/C^2$ vs voltage curve using the relation (1). The variation of $1/C^2$ is shown in the part (c) of fig.8. The charge carrier concentration has been found to be $1.6 \times 10^{14}\ cm^{-3}$.

$$\mathbf{1/C^2=2(V+V_{bi})/q\varepsilon N_{SC}A^2} \quad (1)$$

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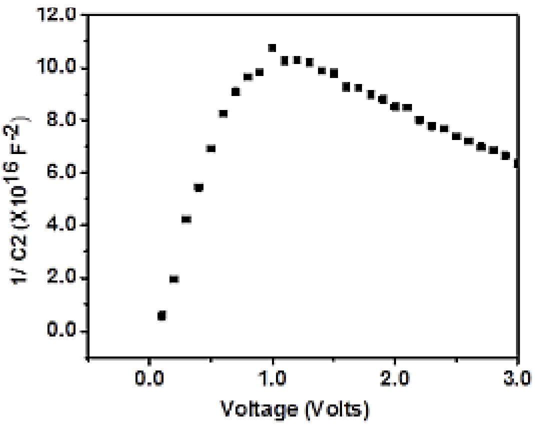


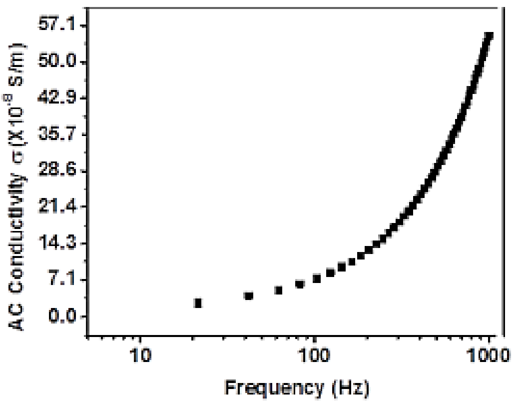
Figure 8: Variation of $1/C^2$ with applied bias voltage

Further to understand the transport mechanism of carriers through the film, AC conductivity of the film was measured over wide range of frequencies. The semi log curve of AC conductivity of the sub pc film is shown in figure 9. The obtained AC conductivities[13] were fitted with universal power law (eq. 2)

$$\sigma = \sigma_0 + A\omega^n \qquad (2)$$

The σ_0 represents the DC conductivity of the film and was found to be 4.2 X 10 $^{-10}$S/m. Further the exponent was found to be equal to 0.63.The exponent in equation (2) is a key parameter

which gives insight into the transport mechanism of carriers through the film. The obtained value of 'n' is less than one corresponding to hopping conduction mechanism through the film.



IV. CONCLUSION

In conclusions we report that sub pc forms amorphous films with average grain size of the order of 200 nm. The real part of complex refractive index show strong depression at560 nm which is in consonance with the absorption UV-Vis spectra. A corresponding peak in imaginary part reaffirms the obtained results. The sub pc film capacitance exhibited typical dielectric relaxation phenomenon with a clear maxima in differential susceptibility curve. The carrier mobility and carrier concentration was found to be 2.6 X 10^{-8}cm^{2}V^{-1}s^{-1} and 1.6X10^{14} cm^{-3} respectively.The transport mechanism was found to be hopping in nature.

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