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Effect of substrate temperature on structural and optical properties of thermally evaporated thin films of $F_{16}CuPc$

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ABSTRACT

Effect of substrate temperature on optical and structural properties of thin films of Hexadecafluorophthalocyanine ($F_{16}CuPc$) has been studied. Thin films of $F_{16}CuPc$ were deposited onto glass substrates using thermal evaporation technique at different substrates temperatures. Structural characterization has been carried using XRD analysis. Average grain size has been found to be increasing with increasing substrate temperature. Optical characterization has been carried out using the absorption spectra, at normal incidence, in range 200-900 nm. Absorption and extinction coefficients of the films so obtained has been evaluated. Both of these have been observed to vary with wavelength. The values of extinction coefficients have been found to decrease with increasing substrate temperature whereas increase in Optical band gap energy, for direct allowed transitions, with increasing substrate temperature has been noticed.

Keywords: Absorption, Extinction Coefficients, Band Gap, Grain Size

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INTRODUCTION

Organic semiconductors are emerging as possible replacements of inorganic semiconductors due to their low cost of production and ease of fabrication [1] . They have the potential for use as flexible electronic devices such as foldable displays etc. [2]. Semiconducting properties of organic semiconductors are due to the presence of conjugated double bonds in their molecular structure. Π orbitals are the most relevant orbitals for optoelectronic properties of organic semiconductors [3]. The flexibility of synthesizing new molecules by changing either the functional groups or atomic arrangement, which in turn induces a change in the electronic properties of new molecules, and hence makes these organic semiconductors attractive candidates for opto-electronic applications.

Metal Phthalocyanines are an important class of materials for opto-electronic device applications. Many metal phthalocyanines have been investigated for different applications such as thin film transistors, photovoltaics and gas sensors [4-6]. Copper Hexadecafluoropthalocyanine is an n -type, air stable, organic semiconductor with applications in field effect devices and photovoltaics. Structural and optical absorption properties in thin film form are important parameters for the suitability for a material for opto-electronic device applications. In the present work the effect of substrate temperature on optical and structural properties of Copper Hexadecafluoropthalocyanine ($F_{16}CuPc$) have been studied.

MATERIALS AND METHODS

High purity Copper Hexadecafluoropthalocyanine ($F_{16}CuPc$) was procured from Sigma-Aldrich (USA). Thin films of $F_{16}CuPc$ were prepared onto pre-cleaned glass substrates using thermal evaporation technique in pressure better that 10^{-5} mbar using thin film vacuum coating unit (Hind High Vacuum, 12A4D). The rate of evaporation was controlled and kept at 2-5 A° per sec. The thickness of the films was monitored using quartz crystal thickness monitor. The thin films were deposited at substrate temperature of 303, 323 and 373K. The optical absorption spectra was obtained using UV-VIS spectrophotometer (Thermo Fisher, Evolution 300) in the range 200-900 nm. X-ray diffractograms were obtained using X'Pert Pro (PAN Analytical) diffractometer using Cu Kα radiation (λ = 1.5A°) in the range 0-30°.

RESULTS AND DISCUSSION

The optical absorption spectra of thin films deposited at different substrate temperatures have been shown in fig. 1. These spectra have been characterized by two major bands i.e. B and Q band, both corresponding to $\pi - \pi^*$ transitions. Absorption coefficient α was calculated from obtained data and band gap was calculated using Tauc's relation [7] ; $\alpha h\nu = B(h\nu - E_g)^n$, where B is band edge parameter and value of n determines the nature of optical transition (n = ½ indicates direct transition and n = 2 indicates indirect transition). Variation between $(\alpha h\nu)^2$ and hν has been recorded in fig. 2. Linearity of the dependence indicates direct transitions. Extrapolating the linear regions to $\alpha h\nu = 0$ gives the value of band gap. Values of band gap calculated for films deposited at different substrate temperatures are listed in table 1. It is found that the optical band gap increases from 3.02 eV for the film deposited at 300 K to 3.1 eV for film deposited at 373 K. This can be related to the increasing crystallinity of the films with increasing substrate temperature. Optical properties of a material depend upon the interaction of the material with electric field of the electromagnetic wave. The extinction coefficient is a measure of damping of the incident wave in the material [8]. The extinction coefficients has been calculated using the relation $k = \alpha\lambda/4\pi$.

Both the absorption and extinction coefficients are found to vary with incident energy. Variation of absorption coefficient with energy is shown in fig.3 while the variation of extinction coefficients with wavelength for films at different substrate temperatures is shown in fig. 4.

X-ray diffraction spectra of the films deposited at different substrate temperatures are shown in fig.5. All the three spectra show a strong peak corresponding to (001) orientation. Intensity of diffraction peaks increases with the increase in substrate temperature. The grain size has been calculated using the Scherrer formula [9]: $D = \lambda/\beta \cos\theta$ where λ is wavelength of X-rays used, β is FWHM and θ is Bragg's angle. Average grain size has been observed to be increasing with the increase in substrate temperature indicating better crystalline films at higher substrate temperature.

Table 1.Variation in band gap energy and grain size with substrate temperature for thin films of F16CuPc

Substrate Temperature (K)	Band Gap Energy (eV)	Grain Size (A°)
300	3.02	278.8
333	3.05	289.2
373	3.10	307.3

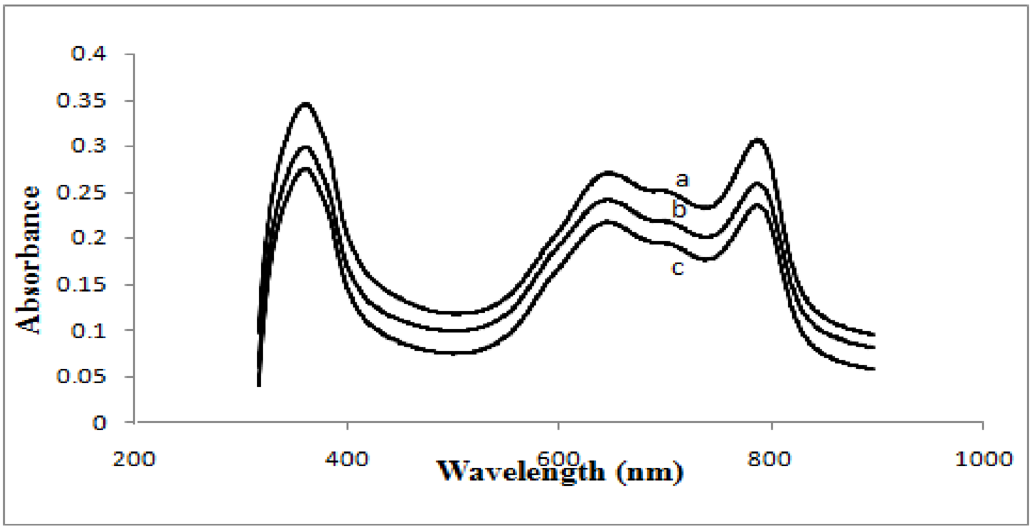

Fig. 1. Absorbance vs wavelength for films deposited (at) 300 K (b) 333 K (c) 373 K

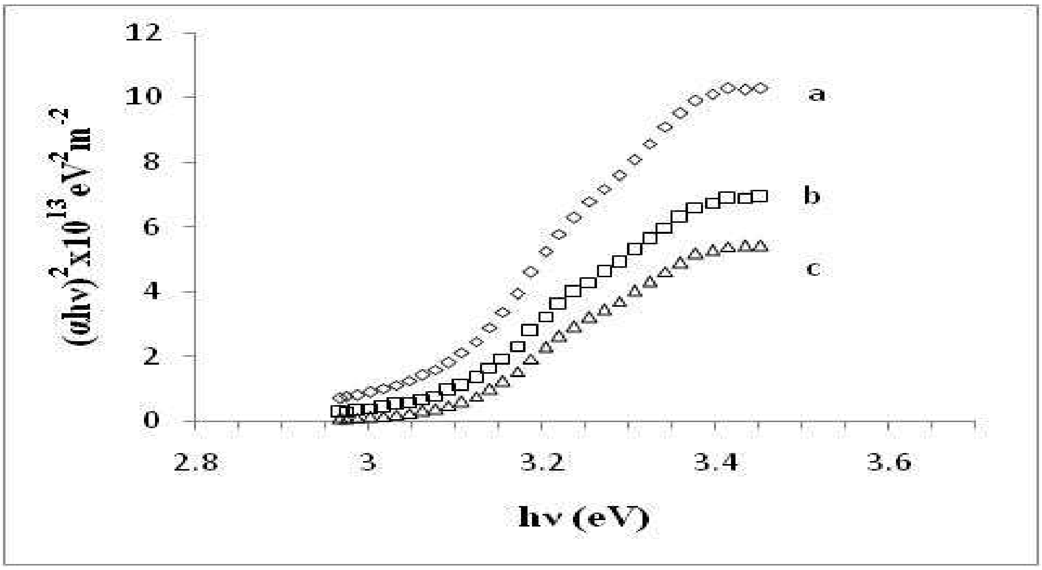

Fig. 2. Variation of $(\alpha h\nu)^2$with hν for films deposited at (a) 300 K (b) 333 K (c) 373 K

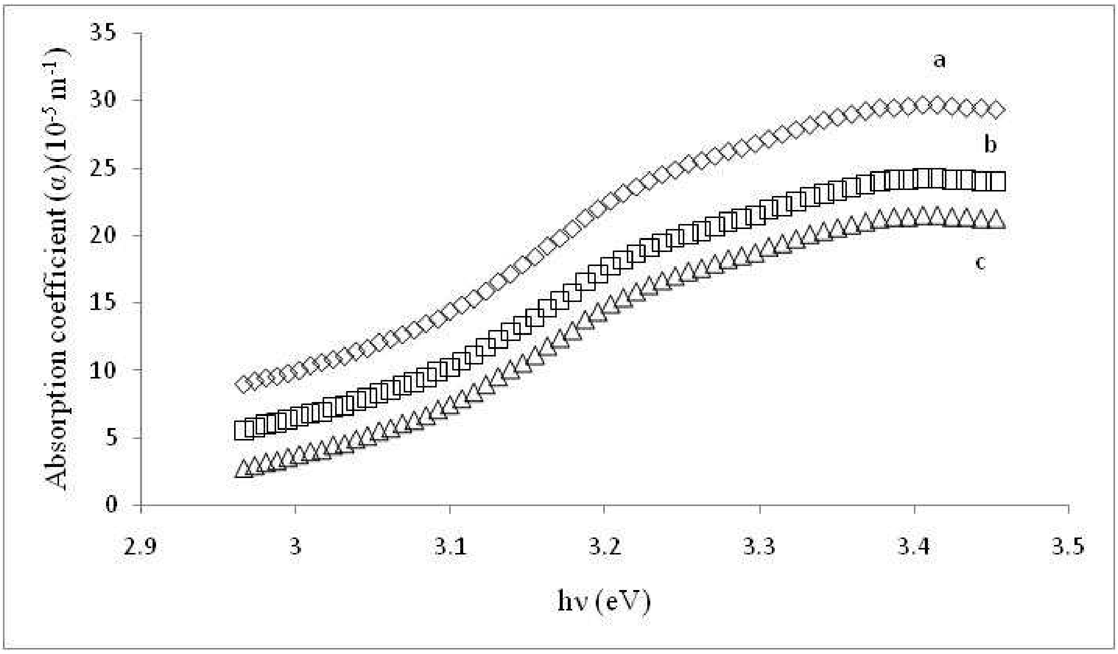

Fig. 3. Variation of absorption coefficient with energy for films deposited at (a) 300 K (b) 333 K (c) 373 K

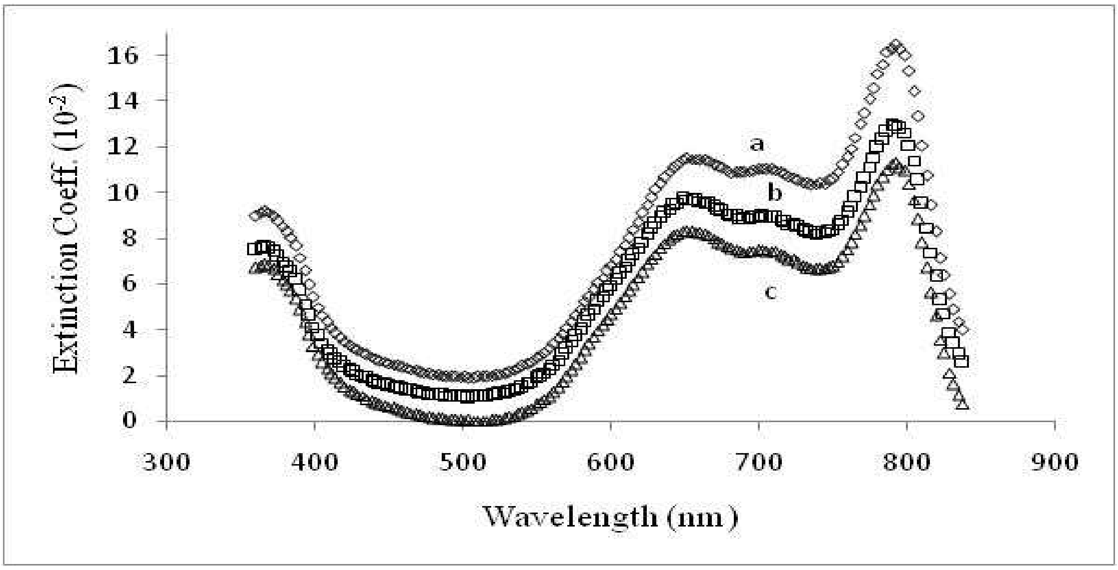

Fig. 4. Variation of extinction coefficient with wavelength for films deposited at (a) 300 K (b) 333 K (c) 373 K

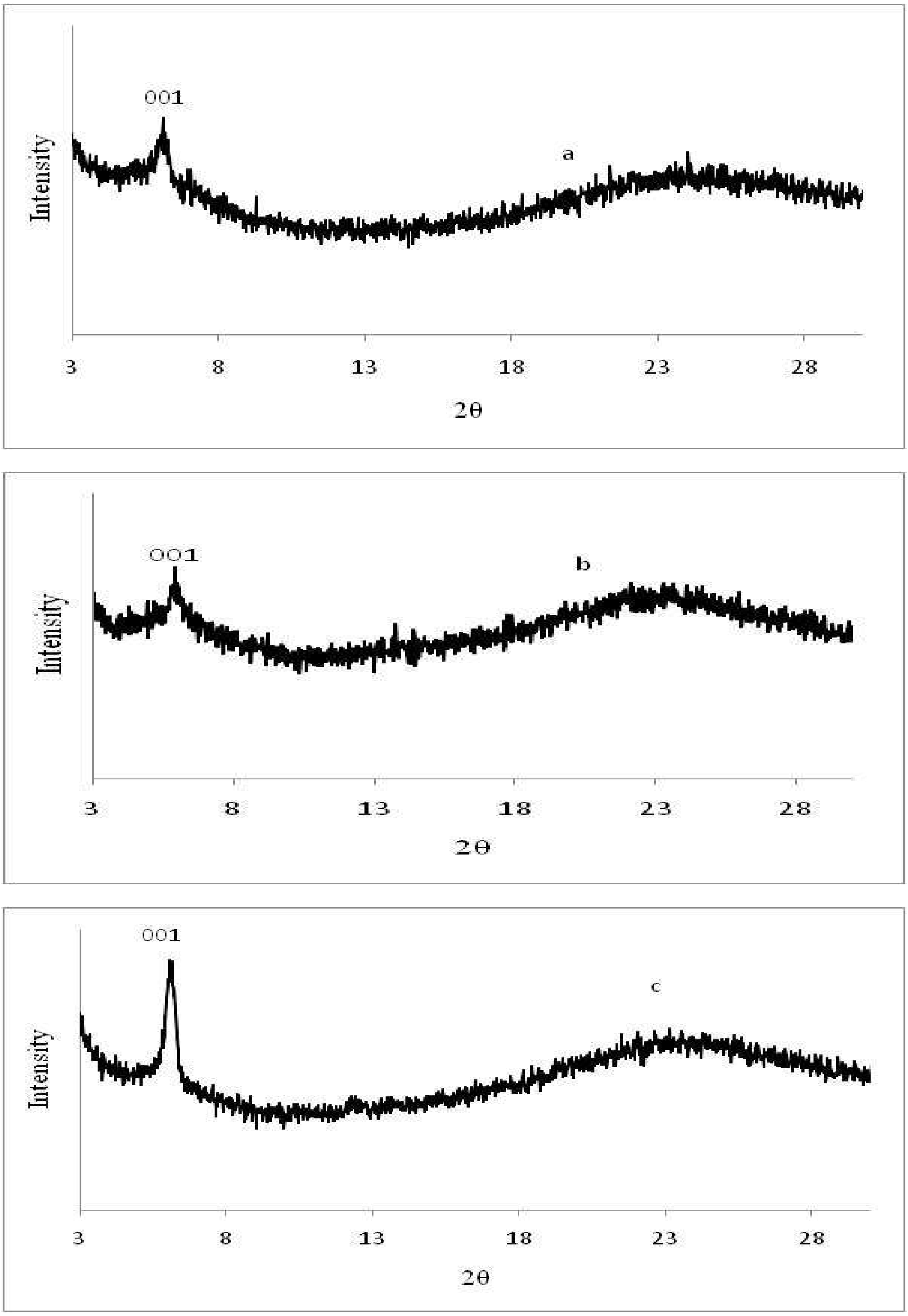

Fig. 5. XRD of F16CuPc thin films deposited at (a) 300 K (b) 333 K (c) 373 K

CONCLUSION

Optical band gap increases with the increasing substrate temperature. Absorption and extinction coefficients vary with wavelength. Extinction coefficients decrease with increasing substrate temperature. Average grain size increase with increase in substrate temperature indicating better crystallinity of films deposited at higher substrate temperature. The optical properties indicate the possible candidature of hexadecafluorophthalocyanine as photovoltaic material.

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