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Determination of optical conductivity and different optical energy losses for non-crystalline Zinc tetra tert - butyl 2,3 Naphthalocyanine thin films

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Abstract

Amorphous Zinc Tetra Tert-Butyl 2, 3 naphthalocyanine thin films (ZTTBNc) have been deposited using Physical Vapor Deposition technique. By analyzing the X-ray diffraction, the structure of as deposited films is found to be non-crystalline. Different optical properties of these thin films have been investigated by means of optical absorption and reflection spectra. From analyzing the optical band gap energy, Eg ; it belongs to wide bandgap type semiconductor. Various optical constants like width of band tails of localized states into the gap, E_U and steepness parameter, β gets calculated and the variation of different optical parameters like refractive index, extinction coefficient, dielectric constants, optical conductivity and surface and volume energy losses with photon energy are estimated.

Keywords: amorphous semiconductor; thermal evaporation; X-ray diffraction; nucleation and growth; optical constants.

1. Introduction

More complex options to porphyrins, Naphthalocyanine have been extensively used as potential materials for optoelectronic and electronic devices for solar cells (Komori et al, 2002). Most studies related to Phthalocyanine derivatives are addressed to the structural aspects of the molecular arrangement in thin films and in solution phase using X-ray photo electron spectroscopy (Kessler et al, 1998). There are little studies on determination of various optical constants of Naphthalocyanine compounds, especially in thin film configuration, even though some optical studies exist (Biswas et al, 2005).

2. Experimental details

Commercially available Zinc Tetra Tert Butyl 2,3Naphthalocyanine (ZnTTBNc) in the powder form, procured from Aldrich Chemical Company (USA) is used as source material for the preparation of thin film.Pre-cleaned micro glass slide of size 75mm×25mm×1.3mm is used as substrate. Evaporation of the material is carried out using Hind Hivac vacuum (Model 12 4A) coating unit at a base pressure of 10^{-5}Torr. Molybdenum boat of dimension 2.9×1.2×0.5cm is used for the evaporation. During evaporation, the substrate is kept at a distance of 12cm from the source. The rate of deposition is adjusted to 1A^{o}/Sec. Thin film of ZnTTBNc is deposited by keeping the substrate at room temperature (303K). The thickness of the film is monitored using quartz crystal thickness monitor and crosschecked by Tolansky's multiple beam interference technique.Structure of as prepared ZnTTBNc thin film is analyzed using Siemans-
EQBCL015 X-ray Diffractometer (Model No. D5005) and optical absorption properties are carried out using CARY 5000 (Version No. 1.09) in double beam mode.

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3. Results and discussions

Xray diffraction analysis of ZnTTBNc thin film having standard thickness of 300nm is having non-crystalline property without any preferred orientation peaks is shown in Fig.1. It reflects the results of different Metal Pcs where the thicker Pc thin films show peaks in the XRD pattern (Pakhomov et al, 2006).

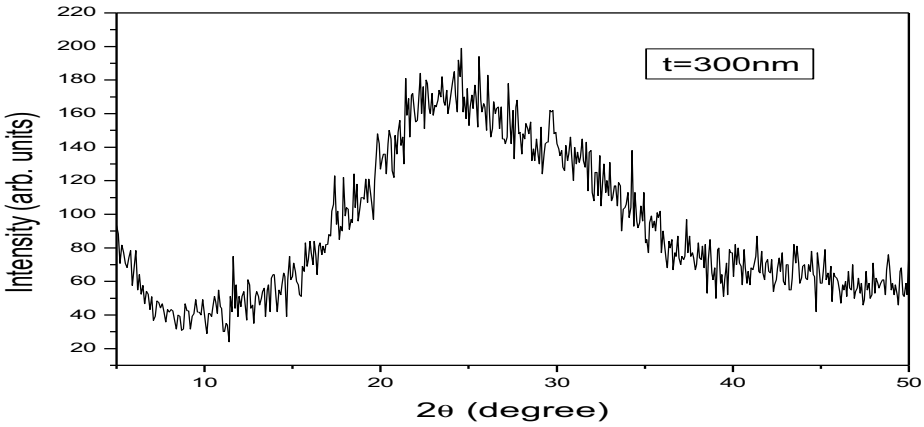

Fig. 1. X-ray analysis diagram of as prepared ZnTTBNc thin film

Optical absorption in infra-red region of ZnTTBNc thin film shows that it is a good NIR emitter. All the relations of optical analysis are taken from (Eom et al, 2005). From the absorbance spectra in Fig.2, the absorption coefficient, α and extinction coefficient, k is determined using the expressions below.

$$\alpha = \frac{2.303 \times A}{t} \tag{1}$$

and

$$k = \alpha\lambda / 4\pi \tag{2}$$

Here the symbols having their usual meaning and different optical constants are tabulated in Table.1.

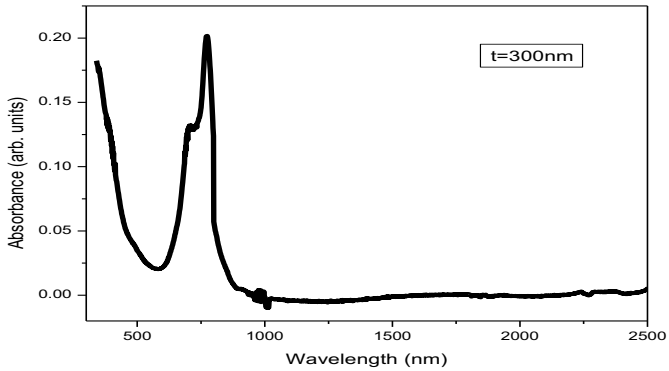

Fig. 2. UV-visible NIR spectrum of ZnTTBNc thin film

Width of localized state in optical bands are determined from equation(3) and Urbach energy E_u for non-crystalline materials and are calculated using the relation (3), tabulated in Table.1.

$$\ln\alpha = \alpha_0 \exp\left[\frac{h\nu - E_I}{E_U}\right] \tag{3}$$

From the Urbach plot, the steepness parameter β can be empirically determined using the relation,

$$\alpha = \alpha_0 \exp\left[\frac{\beta}{KT}(E - E_I)\right] \tag{4}$$

Reflectivity of an absorbing medium of indices n and k in air under normal incidence is given by

$$R = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2} \tag{5}$$

The complex dielectric parameters for VTTBNc thin films are find out using the relation

$$\varepsilon_1 = n^2 - k^2 \tag{6}$$

$$\varepsilon_2 = 2nk \tag{7}$$

Values of ε_1 and ε_2 are tabulated in Table.1. Even though different optical constants have a nonlinear variation with photon energy, they all having their own maximum values and are tabulated in Table.1. Since the material is a photonic one, in addition to electrical conductivity, there is an optical conducting parameter having complex nature and are according to the relation

$$\sigma_1 = \omega\varepsilon_2\varepsilon_0 \tag{8}$$

and

$$\sigma_2 = \omega\varepsilon_1\varepsilon_0 \tag{9}$$

Further the nonlinear variation of surface and volume energy loss with photon energy is plotted in Fig.3.

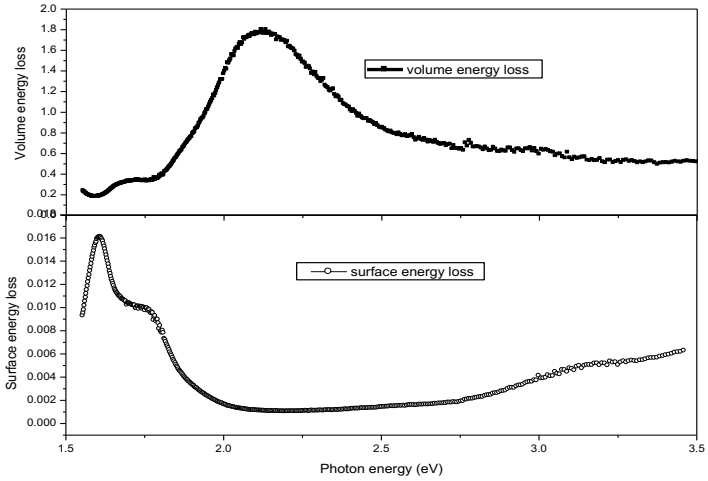

Fig. 3. Variation of energy losses with Photon energy for ZnTTBNc thin film

Volume energy loss

$$\left[-\mathrm{Im}\left(1/\varepsilon\right)\right]=\varepsilon_2/\left(\varepsilon_1^2+\varepsilon_2^2\right) \tag{10}$$

and Surface energy loss

$$\left[-\mathrm{Im}\left(\frac{1}{(\varepsilon+1)}\right)\right]=\varepsilon_2/\left[(\varepsilon_1+1)^2+\varepsilon_2^2\right] \tag{11}$$

ZnTTBNc thin film possesses more intense absorption coefficient peak than that of TTBNc thin film. Here ZnTTBNc thin film having absorption coefficient $\alpha \geq 10^4$ cm^{-1}, the fundamental absorption edge is corresponding to direct allowed interband transitions.

Maximum value of optical parameters for freshly prepared ZnTTBNc thin film		Values obtained
Absorption coefficient (α) × 10^4 (cm^{-1})		15.50
Band gap energy	Eg_1 ±0.01(eV)	2.97
	Eg_2 ±0.01(eV)	1.50
Urbach energy (Eu) ±0.01(eV)		1.85
Steepness parameter (β) × 10^{-2}		1.39
Figure of Merit (ψ_{TC}) ×10^{-2} ($\Omega^{-1}m^{-1}$)		9.66
Extinction coefficient (k)		0.10
Refractive index (n)		2.23
Dielectric constants	ε_1	5.65
	ε_2	0.28
Optical conductivity	σ_1	8.01
	σ_2	18.17
Surface energy loss		0.02
Volume energy loss		1.77

Table .1. Optical parameters for freshly prepared ZnTTBNc thin film (t=300nm±15nm)

4. Conclusions

Amorphous nature of as prepared ZnTTBNc thin film account for X-ray analysis. Addition of central metal atom like Zn apart from hydrogen atom in metal free TTBNc enhances most of the optical parameters in their maximum peak values. Figure of merit for as deposited ZnTTBNc is found to be higher than the metal free and is having a comparable transmittance with ZnO thin films. So, for the fabrication of transparent semiconductors, Zinc substituted TTBNc shows maximum efficiency than the metal free one in its optical characteristics.

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