Materials Science in Semiconductor Processing 38 (2015) 177–183

Contents lists available at ScienceDirect

Materials Science in Semiconductor Processing

journal homepage: www.elsevier.com/locate/mssp

Structural and optical properties of nanocrystalline aluminum phthalocyanine chloride thin films

M.M. El-Nahass [a], H.S. Soliman [a], B.A. Khalifa [b], I.M. Soliman [b,*]

[a] Physics Department, Faculty of Education, Ain Shams University, Heliopolis, Cairo, Egypt
[b] Physics Department, Faculty of Science, Ain Shams University, Abbasia, Cairo, Egypt

ARTICLE INFO

Available online 14 May 2015

Keywords:
Organic compound
AlPcCl thin films
Thermal evaporation
Optical properties

ABSTRACT

Thin films of aluminum phthalocyanine chloride (AlPcCl) were fabricated, with different thicknesses (109–518 nm) using thermal evaporation technique. Structural and optical properties of AlPcCl thin films were investigated. The material in powder form showed a polycrystalline nature with monoclinic structure. Miller indices, *hkl*, values for each diffraction line in X-ray diffraction (XRD) spectrum were calculated. The field emission scanning electron microscope (FESEM) showed the nanostructure property of the as-deposited thin films. The optical properties of the thin films were studied by the spectrophotometric measurements of the transmittance, *T*, and the reflectance, *R*, at the normal incidence of the light in the spectral range 200–2500 nm. The refractive and absorption indices of the thin films were calculated and were found to be independent of film thickness of 109–518 nm. The films exhibited indirect allowed inter-band transitions. The optical band gaps transitions were calculated as 1.42, 2.87 and 3.69 eV, respectively. Also, different dispersion and absorption parameters were determined for thin films of AlPcCl.

© 2015 Elsevier Ltd. All rights reserved.

1. Introduction

Organic semiconducting materials are of particular interest, since they possess a prosperous optoelectronic, electrical and processing properties for designing and fabrication of electronic devices [1]. Among these materials, a series of phthalocyanines represent a large family of heterocyclic conjugated molecules with high chemical stability. Phthalocyanines as a class of organic materials are generally thermally stable and can easily be deposited as thin films with high quality by thermal evaporation without dissociation. Metal phthalocyanines (MPc's) have gained considerable attention in recent years because they have been successfully applied in many applications such as gas sensors [2,3], solar cells [4–6] and light emitting diodes [7,8]. Optical absorption studies of MPc's thin films have attracted the researchers over the last few years [9,10]. Relatively few studies have focused on the halogenated MPc's although there is evidence that they may exhibit properties suitable for gas sensing applications [11]. It has also been shown that the halogenated Pc's exhibit remarkable morphological and thermal stability over a larger temperature range compared to unhalogenated Pc's [12].

One of the most halogenated MPc's derivatives is aluminum phthalocyanine chloride (AlPcCl), which is the focus of our study. It has a chemical formula of ($C_{32}H_{16}AlClN_8$). In the present work, we introduce a detailed study about optical properties of AlPcCl thin films. Studying the optical properties like energy gap has an important role especially in the photovoltaic technology where the efficiency of the devices depends mainly on it.

* Corresponding author.
E-mail address: solidhima@gmail.com (I.M. Soliman).

http://dx.doi.org/10.1016/j.mssp.2015.04.014
1369-8001/© 2015 Elsevier Ltd. All rights reserved.

2. Experimental details

The AlPcCl powder ($C_{32}H_{16}AlClN_8$) was obtained from Sigma- Aldrich Chem. Co. Thin films of AlPcCl with different thicknesses 109–518 nm were prepared by thermal evaporation technique, using a high vacuum coating unit (Edward, E306A). Thin films were evaporated from quartz crucible source charged by AlPcCl and heated by a tungsten coil in a vacuum of 10^{-4} Pa during deposition. The films were deposited onto pre-cleaned quartz substrates maintained at room temperature and the deposition rate was controlled by using a quartz crystal thickness monitor (Edwards, FTM6). Film thickness was determined after deposition by using multiple-beam Fizeau fringes in reflection [13].

The structural characterizations were investigated by using X-ray diffraction patterns (XRD). A Philips X-ray diffractometer (model X'Pert) was used for the measurements utilized monochromatic Cu$K\alpha$ radiation operated at 40 kV and 25 mA. The diffraction patterns were recorded automatically with a scanning speed 2° min^{-1} in the 2θ range. The surface morphology of the AlPcCl thin films was studied by the scanning electron micrograph images obtained from field emission scanning electron microscope model-quanta 250 FEG (FEI-Company). Infrared spectroscopy of AlPcCl in powder and thin film forms was performed using ATI Mattson (Infinity series FTIR) infrared spectrophotometer in the spectral range 4000–400 cm^{-1}. A disk shaped from AlPcCl powder was mixed with vacuum dried grade KBr in percentage of 2:98, respectively. The FTIR measurements for thin films were come out for the films deposited on circular KBr single crystal substrate.

For optical measurements, the transmittance, T, and the reflectance, R, of the films were measured at normal incidence in the spectral range 200–2500 nm using a double-beam spectrophotometer (JASCO, V-570 UV–VIS–NIR). The spectral data obtained directly from the spectrophotometer were transformed to absolute values by making a correction to eliminate the absorbance and reflectance of the substrate. The absolute values of $T(\lambda)$ and $R(\lambda)$ are given by [14]:

$$T=\left(\frac{I_{ft}}{I_q}\right)(1-R_q) \tag{1}$$

where I_{ft} and I_q are the intensities of light passing through the film-quartz system and that passing through the reference quartz, respectively and R_q is the reflectance of the quartz substrate, and

$$R=\left(\frac{I_{fr}}{I_m}\right)R_m(1+[1-R_q])-T^2R_q \tag{2}$$

where I_m is the intensity of light reflected from the reference mirror, I_{fr} is the intensity of light reflected from the sample and R_m is the mirror reflectance. The absorption coefficient, α, the absorption index, k, and the refractive index, n, can be calculated by using the following equations [14–16]:

$$\alpha=\ln\left[\frac{(1-R)^2}{2T}+\sqrt{R^2+\frac{(1-R)^4}{4T^2}}\right] \tag{3}$$

$$k=\frac{\alpha\lambda}{4\pi} \tag{4}$$

$$n=\left(\frac{1+R}{1-R}+\sqrt{\frac{4R}{(1-R)^2}-k^2}\right) \tag{5}$$

where α is the absorption coefficient and d is the film thickness. The experimental error in measuring the film thickness was taken as ±2%, ±1% in T and R and ±4% in the calculated values of n and k [17].

3. Results and discussion

3.1. Structural characterization

The structural properties were investigated for determining the lattice parameters together with a complete list of the Miller indices and interplanar spacing for AlPcCl. Structure examination was carried out by using Crysfire and Chekcell programs [18,19]. These programs were utilized to index all the diffraction peaks, calculate Miller indices (hkl) and the interplanar spacing (d_{hkl}) value for each diffraction peak which estimate the lattice parameters of the investigated compound. The calculated $(2\theta^o_{calculated},\ d_{calculated})$ are the theoretical values for the proposed crystalline system by using Crysfire program, while $(2\theta^o_{measured},\ d_{measured})$ are the real measured data. The XRD patterns obtained for AlPcCl in the powder form shown in Fig. 1(a) indicates that the material is polycrystalline. Applying computer program Crysfire [18] for indexing all the diffraction lines, it was found that the calculated ($2\theta^o$) values, which obtained from the program are in satisfactory agreement with the observed values; therefore, the present deduced indexing can be accepted and the AlPcCl lattice as a monoclinic one with space group P2 with the lattice parameters: a=19.95 A°, b=18.81 A°, c=19.34 A°, $\alpha=\gamma=90°$ and β=118.29°. Table 1 shows the values of Miller indices, (hkl), for each diffraction peak together with the interplaner spacing (d_{hkl}) obtained by using Chekcell program [19]. Fig. 1(b) shows diffraction peaks appeared on the XRD patterns of as-deposited AlPcCl film of thickness 385 nm, and as observed, there are only two significant peaks around 2θ°=25.19° and 31.76°. The SEM image Fig. 2 can be used to assess the surface morphology of the as-deposited AlPcCl film of thickness 385 nm. It shows clearly almost uniform distribution of nanocrystallite particles of 10–28 nm over the entire surface of the sample.

The infrared (IR) absorption technique is used to identify the phase nature of MPc powder as well as thin film, as the IR spectrum is markedly dependent on the chemical composition and its crystalline form [20]. MPcs are known to have different polymorphs that can strongly be identified by IR absorption technique [20–23]. Two polymorphs (α-metastable and β-stable) can occur because of the slight differences in the π–π electronic interaction between the neighbor molecules in the

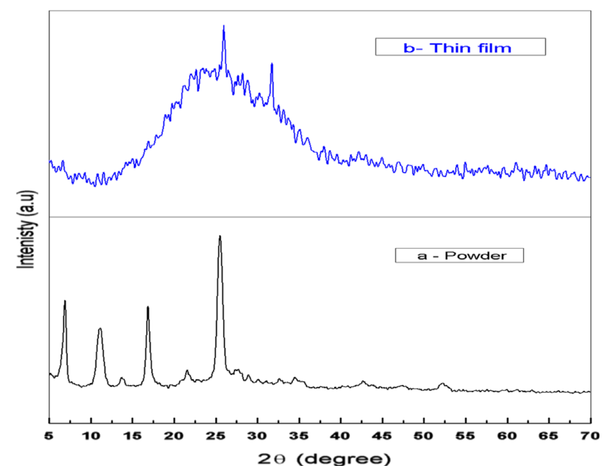

Fig. 1. XRD of AlPcCl in: (a) the powder form, (b) as-deposited thin film.

Download English Version:

https://daneshyari.com/en/article/728300

Download Persian Version:

https://daneshyari.com/article/728300

Daneshyari.com