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An investigation on linear and non-linear optical constants of nano-spherical CuPc thin films for optoelectronic applications

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ABSTRACT

In the current work, the authors present the systematic study on linear and nonlinear optical properties of Copper-phathalocyanine thin film deposited by thermal evaporation system for the first time. The thickness of the prepared thin film was measured and found to be ~300 nm. X-ray diffraction and AFM study confirms that the prepared thin film possess good quality. The orientation of the grown thin film is found to be along (100). UV–vis-NIR study shows that the deposited thin film is highly transparent (>80%) in the wavelength range of 700–2500 nm. Further, the recorded optical data was used to determine the various linear and nonlinear optical parameters. The calculated value of refractive index is found to be in the range of 0.4–1.0. The direct and indirect band gap value is found to be 2.9 and 3.25 eV, respectively. The value of linear and nonlinear susceptibilities is found to be in order of 10^{-12}. The higher value of linear and nonlinear parameters makes it suitable for optoelectronic applications.

1. Introduction

In recent past, the thin films of organic nonlinear optical materials gain much importance due to their wide range of applications in modern technological devices such as memory cards, optical display, optoelectronics, metal–insulator based semiconductors and also in industrial applications like: gas detecting systems [1–6]. The organic semiconductor thin films have large flexibilities than the inorganic counterparts from various aspects such as they possess high charge mobility, high switching speed, large coverage area for display systems, low temperature processing and low cost preparation, which makes them superior than inorganic semiconductors [7–11]. The most important property of these organic materials is that they can easily form bonds with metal ions and produce metal complexes. Moreover, among different organic thin films, phthalocyanine compounds of organic dye, especially metallophthalocyanine derivatives have attracted many researchers and scientists around the world due to their macro-cyclic nature of conjugated π-electrons. Phthalocyanine is one of such important organic dye, when it is mixed with metal ion like copper it become potential candidate for low cost display devices [12], good absorber in UV–vis region and possess high thermal stability [13]. Due to these special features, it seems to be necessary and justified to prepare and study the metal-organic dye of copper-phthalocyanine (CuPc) for future applications. According to the available literature a considerable amount of work has been done on CuPC thin film in which most of the work is reported on their preparation, structural and spectral properties. However, some studies like optical constants of linear and nonlinear coefficients and susceptibilities are still missing in the literature so far. Hence, in the current work the copper phathalocyanine thin film has been deposited by thermal evaporation technique and systematic studies on linear and nonlinear optical parameters like: absorption coefficient, direct and indirect band gap, real, imaginary parts of dielectrics, refractive index and susceptibility has been done using spectroscopic measurements. The obtained results are may be quite useful for device makers and the results of various optical characterizations are discussed in their respective sections.

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2. Experimental details

2.1. Preparation of CuPc thin film

Pure copper-Phthalocyanine (CuPc) was purchased from Sigma-Aldrich Co. and applied in this work without further purification. Edward thermal evaporation system (E-306 A) was used to fabricate the CuPc thin film on highly cleaned glass substrate. The base vacuum pressure of the machine was maintained at 1.5×10^{-5} Torr before starting the deposition of film. The rate of evaporation was fixed at 5 nm per second until reached the 300 nm followed the shutter closing after reaching the required thickness. For the fabrication of CuPC thin film, the required amount was loaded in to a molybdenum boat with a special arrangement on the top with tiny quartz tube with narrow open hole to prevent the escape of material under the heating source.

2.2. Characterization techniques

The prepared thin film is subjected to X-ray diffraction (XRD) study using powder X-ray diffractometer (Shimadzu LabX XRD-6000) of monochromatic $CuK\alpha$ radiation source operated at 40 kV voltage and 25 mA current with constant scanning speed of 2°/min in the angular range of 5–90° for conforming the crystallinity of thin film. Further the various key parameters like: crystallite size, dislocation density and lattice strain are determined. To assess the surface topography and nanostructure of the as-prepared samples, Atomic force microscopy (AFM) study is carried out using NT-MDT (Type Next, Russia) in non-contact mode and the analysis of grain size and film roughness was done using the attached NT-MDT software. UV–VIS–NIR spectrophotometer (JASCO V-570) was used to measure the transmittance, $T(\lambda)$, reflectance, $R(\lambda)$, and absorbance, $abs(\lambda)$ of the CPC thin film, over the wavelength range of 280–2500 nm. All the optical parameters such as absorption coefficient (α), optical band gap (E_g), absorption Index (k), dielectric constant of real and imaginary parts (ε_1 and ε_2), linear and nonlinear refractive indices (n_1 and n_2), SELF, VELF and nonlinear optical properties are calculated from the recorded data.

3. Result and discussions

3.1. Structure properties

A recorded X-ray diffraction pattern of CuPc thin film is shown in Fig. 1(a). From figure it is clearly visible that CuPC film possess single crystalline phase embedded in amorphous matrix. The crystalline peak was located at 6.623° of (100) face clearly indicates the stable crystalline structure of CuPc thin film, which is quite comparable with standard value of β-form CuPc crystal. The existence of amorphous hump from 15° to 30° in XRD data is considered as the concentration of amorphous material inside the CuPc film [14]. Similar peaks was also observed by Puigdollers et al. and Liu et al. at 6.90° and 6.60° respectively [15,16], indicates these values quite near to the present work. Further, Gomez et al. [17] have studied the crystalline structures of various phthalocyanine derivatives and concluded that during the preparation of phthalocyanine compounds in evaporation process, it is very difficult to get highly crystalline structures because of their high surface mobility of molecules on substrate. However, in the present study, we have obtained a single peak with reasonably good intensity assigned to (100) face of CuPC (ICDD Card no. 11-0893), indicates that our film possess better crystallinity than the earlier studied thin film. The crystal system was conformed to be monoclinic with space group P21/a, and calculated lattice parameters are found to be a=19.40 Å, b=4.80 Å, c=14.64 Å, and β=120.57, which are in close agreement with earlier report (ICDD Card no. 11-0893). From observed X-ray diffraction patterns, the grain size of crystallite was calculated from Scherer's equation [24]:

$$D = \frac{0.9\lambda}{\beta \cos \theta}, \tag{1}$$

where D is the grain size of the crystallite, λ is the wavelength of X-rays, β is the broadening of diffraction calculated at the half width of maximum intensity and θ is the angle of diffraction. The calculated value of crystallite size is found to be 5.30 nm, which is explaining high crystallinity of the prepared film. The observed value is quite higher than earlier reported data on CuPc indicates that the present film is of good quality. From the present structural studies, we can also estimate the dislocation density (δ) and lattice strain of the sample by using the following relation [25]:

$$\delta = n/D^2, \tag{2}$$

where n=1, always indicate the minimum dislocation density of film and D is the crystallite size. The dislocation density of the any material provides the information about quality of films and defect structure of material. Usually the dislocation density is defined as the number of dislocations per unit length or per unit area [26]. In present study, the dislocation density of CuPc film is found to be 0.036 nm^{-2}. The lattice strain of the present sample is calculated by using the following formula [25]:

$$\epsilon = \beta \cos \theta/4 \tag{3}$$

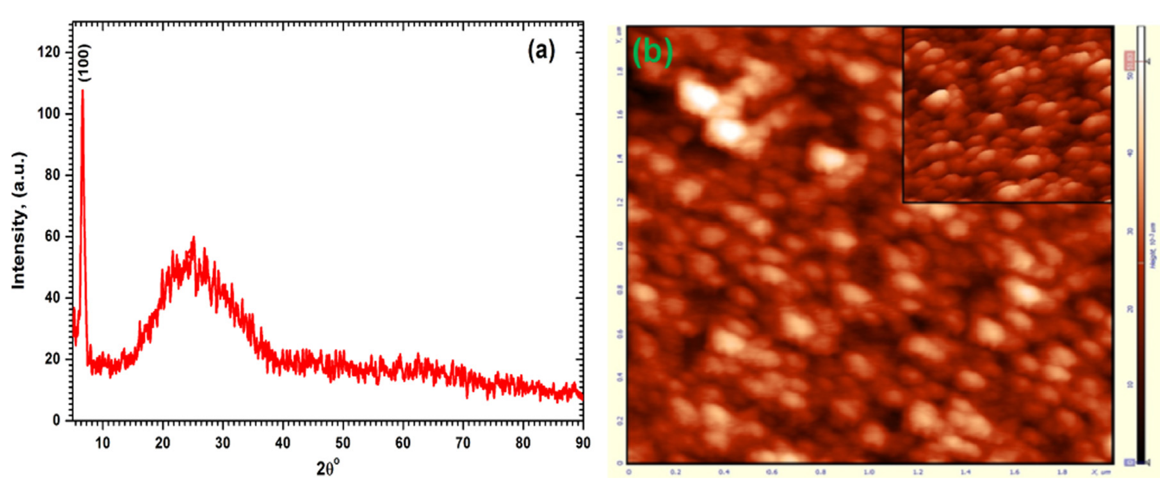

Fig. 1. (a) XRD pattern and (b) 2D AFM micrographs of CuPc thin film.