Materials Letters 205 (2017) 70–74

Contents lists available at ScienceDirect

Materials Letters

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

Preparation of coronene nanowires and its properties

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ARTICLE INFO

Article history:
Received 6 February 2017
Received in revised form 24 May 2017
Accepted 31 May 2017
Available online 1 June 2017

Keywords:
Thin films
Coronene
Organic
Dielectrics

ABSTRACT

In this study we have deposited coronene nanowires onto glass substrates with thicknesses of 80 nm by means of Physical Vapor Deposition (PVD) method and investigated the optical properties of these films. Several parameters such as absorption coefficient, optical and transport band gap, energy of the exciton, real and imaginary dielectric constant and refractive index of the films have been determined using spectrophotometric measurements of transmittance and reflectance. The optical transmittance of the coronene film has been estimated as of 70–90% in the visible range. The optical and transport energy band gaps have been found to be 3.2 and 3.5 eV, respectively. The real dielectric constant and the dielectric loss tangent have significantly increased with photon energy.

1. Introduction

Since technological interest as organic semiconducting materials, polycyclic aromatic hydrocarbons (PAHs) have been attracted significant attention in various scientific groups. These organic compounds are stable with the largest molecular masses [1,2]. A number of such molecules have different optoelectronic properties and can be developed to high-performance organic electronic devices such as thin film transistors (OTFTs), light-emitting transistors (OLETs), light-emitting diodes (LEDs), Schottky barrier diode [3,4] and photovoltaic cells (OPVs) [5–7].

Coronene is condensed polycyclic aromatic hydrocarbon with chemical formula of $C_{24}H_{12}$ comprising six peri-fused benzene rings [8]. It is known also as an interstellar medium as well as an inclusion in the mineral called karpatite [9]. Due to its charge transport mechanism and light-emitting capabilities, coronene draws attention such as rubrene in optical and organic electronics properties [10,11,12].

Many studies have been reported for optical and electrical properties of coronene molecular layers. Xiao et al. [13] have fabricated coronene nanowires by the reprecipitation method using a solution of THF and reported the photoswitching and light-emitting behaviors of these nanowires. Zhang et al. [14] have fabricated the coronene-PVK blends by spin-coating technique and reported this molecular layer as an emitting layer for organic LEDs.

In this paper, we have investigated some optical properties of coronene thin films by using the optical spectra. The surface morphology of coronene films has been characterized by SEM.

2. Experimental procedure

The coronene powder was purchased from Sigma–Aldrich Co. Corning 1737 glass was used as substrate for optical measurement. The glass substrate was cleaned in trichloroethylene, methanol and propanol for 10 min. by using an ultrasonic cleaner. After each cleaning step glass substrates were rinsed with 18 MΩ-cm resistivity deionized water and dried in N_2. The glass substrates were finally cleaned by ultraviolet-generated ozone cleaner before being inserted in the chamber. The coronene powder was thermally evaporated from a special tantalum boat onto glass surfaces in a PVD unit (Nanovak PVD System) with the deposition rates of 0.2 Å/s at about 1×10^{-7} Torr. The temperature of the glass substrate was maintained at 40 °C during the deposition process. The transmittance and reflectance measurements of film were carried out at 300 K with normal incidence of light with the integrating sphere between 200 and 2500 nm in steps of 2 nm using a double-beam photospectrometer (Jasco V-670). The structure was analyzed by Bruker D8 XRD (CuKα source, λ = 1.5406 nm). The surface morphology of the prepared coronene films was observed by Scanning Electron Microscope (SEM, Zeiss Evo-LS10). The accelerating voltage was 20 kV to study the surface morphology of the coronene/glass coated with gold to increase the conductivity. The film thickness measured from the cross section image was about 80 nm from SEM measurements.

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http://dx.doi.org/10.1016/j.matlet.2017.05.137
0167-577X/

3. Results and discussions

3.1. Surface morphological characterizations of coronene thin films

Coronene used in this study has been confirmed by X-ray diffractometer and the result is shown in Fig. 1a. The XRD peaks slightly shifted to lower values fit to standard coronene (PDF no: 00-021-1611) peaks. The coronene shows three intensive peaks centered at 2θ = 11.71°, 12.11° and 18.25° corresponding planes to (002), (−102) and (200), respectively. The sharp XRD peak at 2θ = 11.71° is resulted from the ordered packing of coronene molecules. The distinct peaks have been centered at 2θ = 11.71°, 12.11°, 17.47°, 18.25° and 28.45°. Moreover, any characteristic peaks of other substance have not been detected in XRD pattern which is showed that obtained coronene has a high purity.

The SEM images of coronene nanowires are given in Fig. 1b. As seen in Fig. 1b, the prepared coronene films showed that the whole surface of the substrate is covered by a uniform and smooth distribution of nanowire. Fig. 1c shows the cross-sectional SEM images of coronene films. As seen in Fig. 1c, the crystal structure of coronene nanowires consists of both the smaller and large diameters in the range 50–140 nm.

3.2. Optical characterization of coronene thin films

Fig. 2a depicts the dependence of transmittance and reflectance on the wavelength (λ) of coronene prepared on the glass substrate for the incidence of light between 200 and 2500 nm. As seen from Fig. 2a the coronene thin film shows high transparencies in the visible area whereas the other sides of the transmission show the absorption. The average values of optical transmittance and reflectance in the visible range have been measured ranging from 80 to 90% (for 450–750 nm) and from 9.8 to 5.5% (for 410–700 nm). The sharp drop of optical transmittance is due to the beginning of the basic absorption. At longer wavelengths ($\lambda > 450$ nm) there is no scattered or absorbed light and it is known as non-absorbing region ($R + T = 1$). At shorter wavelengths ($\lambda < 450$ nm) it is known as absorbing region ($R + T < 1$) due to the presence of absorption [15].

The absorption spectra against wavelength in the range 200–2500 nm of coronene thin film is shown in Fig. 2b and indicates one characteristic peak at 300 nm due to interband of π–π∗ electronic transition from the highest occupied molecular orbital (HOMO) to the lowest unoccupied molecular orbital (LUMO) [16].

The band gaps are important parameters of physical properties of thin film materials. They give the basic absorption limits and express the band structures of thin film. The $(\alpha h\nu)^2$ curve against photon energy ($h\nu$) of coronene thin film is plotted (Fig. 3a) to obtain these parameters. As seen in Fig. 3a, the coronene film has two energy gaps. The larger one is called the transport gap energy (E_g^t) that associated with the transport of a single particle in the solid and corresponds to the energy difference between HOMO and LUMO [17,18,19].

The other is the optical gap energy (E_g^{op}) that corresponds to the initial of optical absorption [17] and attributes to the generation of Frenkel exciton [18,20]. The amount of difference between E_g^t and E_g^{op} is corresponds to the binding energy of the exciton, E_B. From the plot, the optical and transport band gap values of the coronene film have been calculated to be 3.2 and 3.5 eV, respectively. The E_B value of coronene film has been determined as 0.3 eV and is compatible with the NiTTP (0.3 eV) [21] and α-sexithiophene (α-6T) (0.4 eV) [22], respectively.

The $ln\alpha$ versus $h\nu$ plot for coronene thin film is shown in Fig. 3b. In the studied energy range, the absorption tail of coronene film has been investigated. In the range of low absorption the absorption coefficient shows an exponential dependence on $h\nu$. This low absorption region is called Urbach spectral tail [23]. As seen

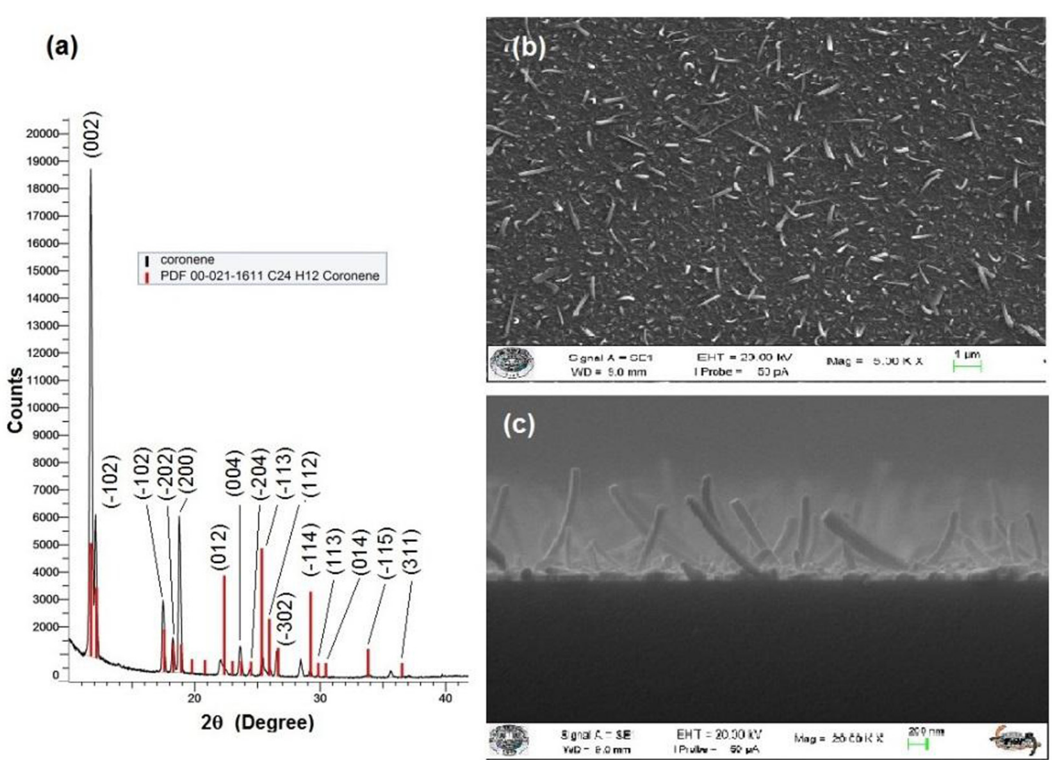

Fig. 1. a) XRD pattern coronene, SEM images: b) surface and c) cross-sectional of coronene nanowires.