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Fabrication and characterization of anthracene thin films for wide-scale organic optoelectronic applications based on linear/nonlinear analyzed optical dispersion parameters

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ABSTRACT

This research work is devoted to studying the linear and nonlinear optical properties of anthracene thin films. For the first time, the fabrication of nanocrystalline anthracene films is presented by using the thermal evaporation conventional technique. All the studied anthracene films exhibit monoclinic crystal structure with dominant preferred orientation along the (001) plane in accordance with X-ray diffraction analysis. The average crystalline size and the strain parameter were calculated and found to be ≈ 14 nm and 42 lines^2. nm, respectively. The transparency of the fabricated anthracene films is high (>80%) from the end of the visible to the near-infrared region at 1500 nm, after that; it reaches to 87%. The characteristic behavior, analysis of refractive index and absorption coefficient based on the measured spectrophotometric data of the transmittance and reflectance spectra. The transition is allowed one and the evaluated optical band gap ~3.1 eV with energy tail ~105 meV. The dispersion curves of the refractive index were found to follow the Wemple-DiDomenico model. The static optical dielectric constant was found to be 2.592. The molecular polarizability of anthracene thin films presented and its value ~56.58 (Å)^3. A simple spectroscopic method is used to characterize and estimate the nonlinear optical susceptibilities. Thermal evaporation technology could be useful to fabricate blue OLED and window film in photodetector devices based-anthracene films.

1. Introduction

There were a lot of efforts in the field of emerging organic semiconducting materials in form of nanostructured thin films with a valuable physical characteristic behavior [1–3]. Towards this trend, the researchers aim to encourage and improve the fabrication and production of low cost transparent and/or semi-transparent ultra-thin organic optoelectronics [3–5]. The scientists and engineers have attempted during the last few decades especially, in fabrications of optoelectronic to decrease the raw material prices and to use simple and cheap fabrication technologies with high-quality products [3–7]. The manufacturers of thin films can fabricate organic films under conservation of its molecular structure by simple technologies with less percolations than that of inorganic thin film fabrication technologies [9,10]. The inorganic films require a lot of considerations and preparation conditions such as: high-vacuum media and high substrate temperatures [8–11]. It is known that the organic films offer good compatibility with plastic, glass, and silicon substrates. In last few years, there is a rapid and continuous increasing in the physical, chemical characterizations and investigations in the field of organic semiconducting films. As a result of this trend; the extensive industrial applications of ultra-thin electronic devices are being recent, a key subject in investments and industries which depending on the advances in nanotechnology [12–14]. Moreover, the ability and processing relative ease of organic semiconducting dyes to be tailored and molecularly engineered with a large variety

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of chromophores for the exogenous variables that stimulate photonic functions in a desirable manner [8–11]. In the fabrication of waveguides [15] and photonic-crystal devices [5,17,18]; the silicon-on-insulator is considered for several decades as a foundation base for photonics fabrication. The replacement of silicon by an organic semiconductor in integrated optical circuits applications is a good target to decrease the costs of research and the photonics industry [16,18].

The prosperous progress of organic/inorganic optoelectronic (photodiodes and solar cells) applications, strongly, depends on the crystal structure, photonic and electrical properties of promising organic semiconducting and dielectric materials. The materials with unique properties; give the research developing team the ability to choose a suitable application before the fabrication process optoelectronic devices. According to this trend, many researchers have tried to fabricate hybrid (organic/inorganic) photonic devices with fast optical signal processing [15–17]. The photon-information transmission (organic/inorganic) devices require molecular organic materials with unique optical functionalities, such as nonlinear ones in particular; second-order $\chi^{(2)}$, and third-order $\chi^{(3)}$, nonlinear optical susceptibility. These parameters are sensitive and measurable for all-optoelectronic ON/OFF and wavelength conversion devices [18–21].

The linear and non-linear optical susceptibilities (such first-order $\chi^{(1)}$, second-order $\chi^{(2)}$, and third-order $\chi^{(3)}$ nonlinear) have special and unique categories due to the molecular structure of an organic material in a crystal. That because, it depends not only on the polarizability of the electrons in the π-bonding orbital but also, on the crystal lattice components (atoms, molecules) contribution. This unique property of organic materials is due to the weak intermolecular bonding on the molecular level, such as interatomic, interaction among dipoles and H-H forces. In addition to weak interactions virtue between these components [20–24]. Looking further ahead, higher efficiency nonlinear interactions could be obtained by using tight spatial confinement of the optical modes [20], from the use of highly nonlinear organic materials [19].

The oligomer electroluminescence materials such as the compounds based anthracene are providing an opportunity to invent almost unlimited adopted host-guest OLEDs systems with a large spectrum of novel interface properties such for photochromic applications [4,8,13]. Anthracene is the parent substance of a large class of dyes and pigments and it's π-electrons cloud overlaps make it behaves like p-type semiconductor [12,16]. Despite the suitability of anthracene in constructing blue emitting materials, in addition to the toggling of its derivatives in much outstanding high photoluminescence yields. As far as the authors know there is a lack in literature survey on the spectrophotometric studies on anthracene thin films based on the measured transmittance and reflectance at normal incidence.

In this work, the authors present in details (for the first time) a spectrophotometric (linear/nonlinear) optical analysis of anthracene thin films and interpreted the linear molar extinction coefficient, band gap, the complex dielectric and nonlinear optical constants. Furthermore, a simplified spectroscopic method is verified and correlated to estimate some important nonlinear parameters. The investigated data were analyzed with the miller relation and the extracted dispersion energy parameters based on (Wemple-DiDomenico) single oscillator model for the fabricated anthracene nanostructured thin films.

2. Experimental details

2.1. The manufacturing method of anthracene thin films

The raw material (where $M_w = 178.234$ g/mole is the molecular weight of anthracene, $\rho_m = 1.25$ g/cm^3 is the density of mass) was imported from Sigma-Aldrich Company. Anthracene films were manufactured on glass substrates by using thermal evaporation technique (Model: Edward, E-306 A, England). The manufacturing process includes two steps as follows:

2.1.1. Substrate cleaning stage

For eliminating dust and any contaminations from the surface of all substrates, all glass substrates were immersed in chromic acid for 10 min and then washed several times by using distilled water. After that, all substrates were rinsed in isopropyl alcohol. There are two steps were done in sequence; firstly: dry nitrogen gas was used to dry the glass substrates and secondly, by using atomic bombardment cleaning option in the first stage of the evacuation process. Finally, the glass substrates were cleaned and ready for the film growth process.

2.1.2. Technological stage of thin film growth

Firstly, the powder was charged in a conical quartz crucible, and the substrates were fixed on the substrate holder inside the machine at 21 cm. After reached the required pressure 1.5×10^{-5} torr, The filament current was switched on to flow through the filament (tungsten coil). At the same time, the temperature of the coil was started to grow up and the crucible itself was heated. As the sublimation temperature was reached (which was determined, previously, with the help of DTA-investigations for anthracene powder), the shutter was switched off and the anthracene films were grown with growth rate ~ 1 nm/s. The growth rate was calibrated many times before the final fabrication process with an original thickness monitor (Model-FTM4) which had fabricated especially for the thermal evaporation coating system model E-306 A.

2.2. Devices and measurements

Differential thermal analyses (TGA/DTA) of anthracene in powder form were measured from 25 to 550 °C) using TGA-50 and DTA-50 (Shimadzu Company).

The crystal structural characterization of anthracene in powder/as-grown films was investigated using X-ray diffraction (XRD-Machine, model X'-pert, operated at fixed applied high voltage ~ 40 kV) and the characterizing monochromatic wavelength = 1.54056 Å; which obtained at current ~ 25 mA of the CuK_α-target.

The topographical characterizations of anthracene films were analyzed with the aid of scanning electron microscopy (model: Philips-XL30).

Spectrophotometric measurements of anthracene films at normal incidence of the light were evaluated in the spectral range 200–2500 nm by spectrophotometer JASCO (model V-570).

3. Result and discussions

3.1. Thermal and structural characteristics of as-grown anthracene nanocrystalline films

Fig. 1 shows the obtained thermally analyzed data by (TGA/DTA) of anthracene powder under a heating rate of 10° C/min to estimate the sublimation temperature of anthracene powder. We can extract from these curves that; the Anthracene is, thermally, stable up to ~177 °C [16,25], the temperature overflow (up to weight loss detection ~ 219.6 °C) the anthracene sublimation phase starts up. At temperature~250 and 277.5 °C, anthracene sample lost a half and full of its initial weight, respectively. The exothermic temperature T_f is correlated with the sublimation of anthracene material.

The experimental XRD data of powder and as-grown films of