Superlattices and Microstructures 64 (2013) 58–69

Contents lists available at ScienceDirect

Superlattices and Microstructures

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

Optical characterization of nano-pentacene thin films

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ARTICLE INFO

Article history:
Received 13 April 2013
Received in revised form 22 July 2013
Accepted 22 August 2013
Available online 4 September 2013

Keywords:
Organic semiconductor
Nano-crystalline pentacene
Thermal evaporation
XRD
Optical dispersion parameters
Optical constants
Optical conductivity

ABSTRACT

The optical properties of pentacene thin films prepared by thermal evaporation technique at room temperature are investigated. X-ray diffraction and atomic force microscopy on the samples showed the existence of the nanostructure in the evaporated pentacene films. Optical properties were studied for the pentacene thin films with various thicknesses (119, 225, 380, and 520 nm) at normal incidence of light in the wavelength range of 300–2600 nm. The refractive index n and the absorption index k were computed using the obtained data of transmittance $T(\lambda)$ and reflectance $R(\lambda)$. The complex dielectric constant, dissipation factor tan δ, optical conductivity σ_{opt}, optical band gap E_g^{opt}, volume energy loss (*VELF*), and surface energy loss (*SELF*) functions were calculated and interpreted. The results of the optical absorption data showed that pentacene thin film has mainly three indirect energy gap bands in the energy range from 1.70 to 3.45 eV. The obtained results indicate that the pentacene organic semiconductor thin film is a good candidate in optoelectronic devices based on its band gap and dispersion parameters.

1. Introduction

Organic semiconductor devices have many advantages such as merit of low-cost, flexibility, and easy technology of fabrication. Therefore, these devices have recently attracted a great deal of interest

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0749-6036/$ - see front matter
http://dx.doi.org/10.1016/j.spmi.2013.08.022

by scientists and engineers alike [1–10]. Pentacene is one of the most promising organic semiconductors, specially, for organic-thin film transistors (OTFTs) because of its good semiconducting properties. Structurally it represents a kind of small molecule, which is consisting of five aligned condensed benzene rings. Such structure allows for pentacene high field-effect mobility that is superior in comparison to other organic semiconductors, generally reaching 1.5 cm^2/Vs. The mobility of single crystal pentacene could increase to 58 cm^2/Vs at 225 K and it is 35 cm^2/Vs at room temperature [11]. Such property makes pentacene one of the ideal materials for fabricating the organic semiconductor devices. Pentacene have been widely used in organic field effect transistors (OFETs) [12–14], organic light-emitting diodes (OLEDs) [15] and organic solar cells [16,17] as an active layer. The possible use of pentacene thin film phototransistors in organic optoelectronic integrated circuits such as interfaces between switches and logical circuits, relay command, transmission of an analogical signal, interfaces between industrial systems and numeric circuits was studied and stated by El Amrani et al. [18]. Moreover, Zhang et al. [19] reported that the introduction of the nanostructural pentacene interlayer have clearly improved the short circuit current density and the power conversion efficiency of a polymer solar cell. In particular, Zhang et al. have observed that for a polymer solar cell integrated with a nanostructural thin film of pentacene interlayer an increased of the cell's power conversion efficiency for about 100% were seen. Such improvement was thought to be related to the short circuit current density.

The objective of this study is to investigate the structural and optical properties of pentacene thin films prepared with various thicknesses (119, 225, 380, and 520 nm). Hence, the absorption spectra are measured in the wavelength range 300–2600 nm. In addition, the optical constants, refractive index *n*, and the extinction coefficient *k*, over the spectral range are determined from the transmittance $T(\lambda)$ and the reflectance $R(\lambda)$. The complex dielectric constant, the volume energy loss and the surface energy loss functions are computed. The dissipation factor and optical conductivity characteristics are calculated as well. Moreover, the energy gaps of the pentacene thin film are also estimated.

2. Experimental procedures

Pentacene was obtained from Sigma Aldrich company (pentacene sublimed grade, ⩾99.9% trace metals basis) and was used without any further purification. Molecular structure of pentacene is shown in Fig. 1. Pentacene films of different thicknesses were prepared via thermal evaporation system (Edward's 306-A) under base pressure of 2×10^{-5} torr. The distance between the glass substrates and the heated silica tube crucible approximately equals 21 cm which is not allowing the heated flow to reach the substrates. The film thickness was controlled using digital quartz crystal thickness monitor attached to the evaporation machine. The deposition rate of the evaporated organic pentacene were about 12–15 Å/s.

X-ray diffraction measurements were taken by an analytical X'Pert Diffractometer System, which has Cu Kα as a radiation source of wavelength λ = 1.540598 Å. The X-ray tube voltage and current were 40 kV and 30 mA, respectively. The 2θ range is 4–80° with a step size of 0.02 and scanning time of 0.4 s.

The transmittance $T(\lambda)$ and reflectance $R(\lambda)$ spectra of the as-deposited pentacene thin films of different thicknesses were measured at normal incidence of light in the spectral range of 300–2600 nm using a double-beam spectrophotometer (JASCO model V-670 UV–VIS–NIR).

The morphology images of the pentacene thin films were investigated by Park System XE-100E atomic force microscopy (AFM) attached with analysis software.

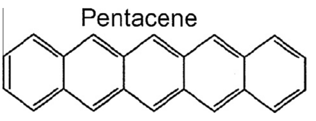

Fig. 1. The molecular structure of pentacene.