Measurement 44 (2011) 1468–1474

Contents lists available at ScienceDirect

Measurement

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

Utilizing a simple and reliable method to investigate the optical functions of small molecular organic films – Alq3 and Gaq3 as examples

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ARTICLE INFO

Article history:
Received 17 March 2011
Received in revised form 20 May 2011
Accepted 26 May 2011
Available online 1 June 2011

Keywords:
Small molecular organic
Gaq3
Alq3
Organic thin film
Optical function
Optical measurement

ABSTRACT

This work reports on the optical functions of tris(8-hydroxyquinolinate) gallium and aluminum small molecular organic films grown by utilizing a home-made thermal evaporator and studied with a spectrophotometer. The non-dispersive refractive index of the Gaq3 and Alq3 films was calculated as 1.77 and 1.68, respectively. The higher refractive index of Gaq3 was attributed to the higher molecular packing density of Gaq3 compared to that of Alq3. A larger dielectric constant for Gaq3 was noticed, indicating the presence of a higher density of states and space charge accumulation in the Gaq3 films compared to those of Alq3. We assigned the presence of direct allowed transition to energy gaps of 2.80 eV and 2.86 eV for the Gaq3 and Alq3 films, respectively. These differences are thought to be caused by the effects of central metal cations of Ga^{3+} and Al^{3+} on their molecular quinolinate ligands.

1. Introduction

Research progress in organic electronics technology has promoted small molecular organic electroluminescent materials [1] to receive considerable attention for their potential application in organic light emitting diodes (OLED) and flat panel displays [2,3]. Since its introduction up until now, tris(8-hydroxyquinoline) aluminum (Alq3) has been the most widely used material for electron transport and emitting layers in fabricating OLEDs [4,5]. A number of theoretical [6,7] and experimental studies [8–13] focused on Alq3 and its derivatives [14,15] to understand and improve their optical properties, in this way realizing long term stable and high luminance OLED devices. However, a different OLED based on Gaq3 [16] has recently shown better performance compared to that of Alq3-based OLEDs prepared under the same conditions. So far, few experimental studies on Gaq3 films have been presented in the literature [17–19]. Moreover, the utilization of Alq3 as buffer electron transport layer (ELT) [20] and dopant material into the donor and/or acceptor layers [21] in organic solar cells (OSCs) has been described. It was found that using Alq3 in OSCs led to an increase in both efficiency and stability of these devices [20,21]. The technological progress in the production of small molecular organic materials for optoelectronic applications, with Gaq3 and Alq3 as major candidates, indicates the need for studies into materials analysis as well as devices fabrication and characterization. The study of the optical behavior of such materials in thin film form [10,22] is a prerequisite for the successful device fabrication. Based on the nature of the films and materials, various methods can be used to estimate the optical parameters, including thickness measurement and monitoring [23–31]. There are some complexities and high costs involved in the existing common techniques used for depositing organic films and their characterization processes [11,13,32]. Interestingly, however, the promising results in the formation of smooth and homogenous films by using relatively low vacuum pressure [17] have inspired this research study to utilize

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doi:10.1016/j.measurement.2011.05.017

a cheap and easy-to-handle, home-made thermal evaporator for investigating the optical parameters of Gaq3 and Alq3 films. When characterizing thin films, it is not always required to control the thickness during the coating process [23]; alternatively, the thickness can be measured after the deposition process. Thus, the current paper reports the investigation of optical functions of Gaq3 and Alq3 films within a wide range of wavelengths (200–2500 nm) by utilizing a simple and reliable method. This method involves a home-made thermal evaporator as the deposition technique and a spectrophotometer for the raw data collection for further numerical operations. The advantages of this method are its fast and simple application for the characterization of small molecular organic films, its low cost, and its reliability.

2. Materials and methods

Tris (8-hydroxyquinolinate) Gallium (Gaq3) and aluminum (Alq3) were purchased from Sigma–Aldrich in powder form and used as received. The molecular structures of the materials in their linear molecular formula of $M(C_9H_6NO)_3$, where M = Ga or Al, and having three ligands each with a phenoxide and pirydyl side group, are shown in Fig. 1a. Fig. 1b shows the schematic diagram of the absorbent organic films deposited onto the transparent quartz slides, while Fig. 1c depicts the schematic of the home made thermal evaporator utilized to grow the investigated films. Films of Gaq3 and Alq3 were sequentially deposited onto the pre-cleaned quartz slides using the home-made thermal evaporator under a base pressure of about 10^{-4} mbar. Initially, powder of Gaq3 or Alq3 was placed inside a quartz boat that has been surrounded by a tungsten coil capable of supplying sufficient heat to the materials upon passing the electrical current through this coil. Currents of about 30–35 A were enough to start sublimating the powders. The quartz substrates were kept at the top of the chamber at room temperature (300 K) during the vapour application and throughout the whole deposition process. Prior to deposition, the quartz slides were cleaned ultrasonically for 15 min with Deacon® Neutracon foam solution, followed by 10 min rinsing in an ultrasonic bath in acetone, ethanol and distilled water, respectively. Finally, the quartz slides were dried thoroughly under nitrogen gas. Quartz slides were selected for this study because of their high optical transparency to just below 200 nm. The optical absorption and transmittance spectra of the films were recorded using a Jasco V-570 UV–Vis–NIR spectrophotometer in the wavelength range of 200–2500 nm. All the measurements were performed under ambient conditions and at room temperature.

3. Results and discussion

From the recorded transmittance data, it is possible to measure the accurate thickness of the films under investigation. Fig. 2 shows the representative transmittance spectra with clear interference fringes that can be seen along the spectral curve. These fringes are due to the optical interference phenomena between the wave fronts created at the two interfaces (air and quartz substrate), which define the sinusoidal behavior of the curves in the region of high transparency. Since the films exhibited a good transparency in the visible and infrared region, the envelope method was chosen as a sensitive tool to determine their thickness. To do this, the refractive index for the films was first calculated at various wavelengths along the envelope (see the zoomed part of Fig. 2), by fitting the transmission maxima and minima of the interference fringes, T_{max} and T_{min}, using the expression [17]:

$$n = \sqrt{N + \sqrt{N^2 - S^2}} \tag{1}$$

where

$$N = 2S\left(\frac{T_{max} - T_{min}}{T_{max} \times T_{min}}\right) + \frac{S^2 + 1}{2} \tag{2}$$

and S is the refractive index of the quartz substrate. T_{max} and T_{min} are tangents to the upper and the lower parts of the transmittance envelope, respectively. In Fig. 2, the arrows show the position of these maxima and minima along the transmission curve.

The interference maxima shown in Fig. 2 can be used to determine the optical thickness nt of the films, where

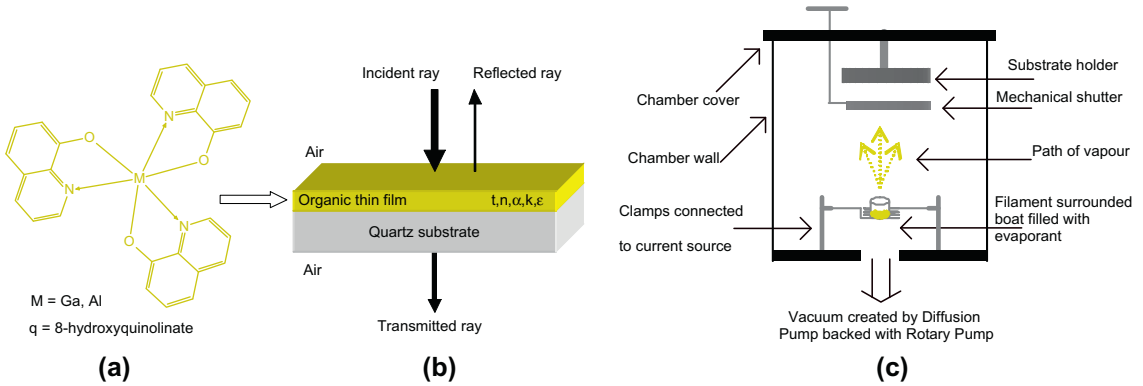

Fig. 1. (a) The chemical structure of Mq3 (M = Ga, Al and q = 8-hydroxyquinolinate), (b) the schematic diagram of the deposited organic films on the transparent quartz slides for the purpose of spectroscopic measurements, and (c) the schematic diagram of the thermal evaporator set-up for thin film deposition.