Journal of Alloys and Compounds 507 (2010) 112–119

Contents lists available at ScienceDirect

Journal of Alloys and Compounds

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

Structural and optical properties of Tris(8-hydroxyquinoline) aluminum (III) (Alq_3) thermal evaporated thin films

M.M. El-Nahass, A.M. Farid*, A.A. Atta

Physics Department, Faculty of Education, Ain Shams University, Roxy, 11757 Cairo, Egypt

ARTICLE INFO

Article history:
Received 6 July 2009
Accepted 14 July 2010
Available online 22 July 2010

Keywords:
Optical properties
Organic materials
Alq_3
Structural properties

ABSTRACT

X-ray diffraction (XRD), transmission electron microscope (TEM) micrographs and optical properties of Tris(8-hydroxyquinoline) aluminum (III) (Alq_3) have been studied. XRD of powder Alq_3 showed that the material has a polycrystalline nature with triclinic structure. The crystal structure and morphology of the as-deposited and annealed (at 473 K for 2 h.) Alq_3 thin films indicated that the as-deposited film is amorphous in nature, while the annealed film has a polycrystalline nature with amorphous background. The molecular structure of the Alq_3 was confirmed by the analysis of (FTIR) spectra. The optical constants such as the refractive index, n, the absorption index, k and the absorption coefficient, α, of both the amorphous and polycrystalline Alq_3 films were determined using spectrophotometric measurements of transmittance (T) and reflectance (R) in the wavelength range (200–2500 nm). The analysis of the data showed an indirect allowed transition energy gaps E_g^{ind} of 2.66 eV and 2.28 eV for the as-deposited and the annealed Alq_3 thin films, respectively. As well as another probability of direct allowed transition was carried out with energy gaps Eg_1^d of 2.82 eV, and Eg_2^d of 4.14 eV for the as-deposited film and Eg_1^d of 2.59 eV, Eg_2^d of 3.88 eV for the annealed films, respectively. Some optical parameters namely molar extinction coefficient (ε_{molar}), oscillator strength (f) and electric dipole strength (q^2) have been evaluated. According to the single oscillator model (SOM), some related parameters such as oscillation energy (E_0), the dispersion energy (E_d), the optical dielectric constant (ε_∞), the lattice dielectric constant (ε_L) and the ratio of free carrier concentration to its effective mass (N/m^*) were estimated. Graphical representation of both the surface and volume energy loss functions and the real optical conductivity as a function of photon energy supports the existence of the mentioned optical transitions.

1. Introduction

Alq_3 enjoys more and more popularity among scientists due to its interesting optical and electrical features like strong luminescence, high electric conductance, low cost and simple technology of fabrication [1]. Therefore, this material is very important in optoelectronic applications such as, photo-detectors OLEDs, flat and flexible color displays and photovoltaic cells.

It is well-known that octahedral complex of the type MN_3O_3, where M is a trivalent metal and N and O stand for the nitrogen and oxygen atoms, respectively, in the quinoline legends, can occur in two different geometric isomers: meridional and/or facial [2].

Three insoluble crystalline phases of Alq_3 namely α-, β-, and γ-Alq_3 have been synthesized [3]. Possibility to design high-luminance low-voltage driven device based on Alq_3 was demonstrated at 1987 [4]. Since that time an intense effort has been dedicated to develop and improve organic electroluminescence diodes (OLEDs) [5]. Alq_3 is a stable material that can be sublimed to grow thin films on large area plastic substrates and stands as one of the most successful materials used in organic electroluminescence applications. Most of the recent studies have been devoted to optimize the device characteristics [6], to improve the morphological stability [7,8], for the understanding of the charge-transport mechanisms [9,10] as well as for tuning of the organic light emitted diode (OLED) emission spectrum [11,12]. Few studies have been devoted to the optical properties of Alq_3, focusing mainly on the solution and sublimed thin film photoluminescence. The aim of the present work is to study the structural and optical properties of thermal evaporated Alq_3 thin films and to deduce the optical parameters using spectrophotometric method of the as-deposited and annealed films. Also, the type of transition is to be identified.

2. Experimental procedure

2.1. Preparation of thin films

The Alq_3 powder used in this study is obtained from (Aldrich). Thin films of Alq_3 of average thicknesses (239 nm) were deposited by thermal evaporation technique, using a high vacuum coating unit (Edwards, E306A). The powder Alq_3 was sublimed

* Corresponding author. Tel.: +20 202 22876569.
E-mail address: ashganfarid@hotmail.com (A.M. Farid).

0925-8388/$ – see front matter © 2010 Elsevier B.V. All rights reserved.
doi:10.1016/j.jallcom.2010.07.110

Table 1
Absorption frequencies in 400–2000 cm^{-1} infrared region for powder, as-deposited and annealed thin film of Alq_3.

Powder $(cm)^{-1}$	As-deposited films $(cm)^{-1}$	Annealed films $(cm)^{-1}$	Assignment
1603.52	1603.52	1603.52	Aromatic C=C bending
1578.45	1578.45	1578.45	Aromatic C=C bending
1498.42	1499.38	1498.42	Aromatic C=C bending
1467.56	1466.6	1467.56	Aromatic stretching C=C
1425.14	1426.1		Aromatic stretching C=C
1381.75	1382.71	1382.71	Aromatic amine
1329.68	1327.75	1328.71	Aromatic amine
1280.5	1279.54	1280.5	Aromatic amine
1230.36	1229.4	1231.33	C–O strong stretching
1176.36	1175.4	1173.47	C–O strong stretching
1113.69	1113.69	1113.69	C–O strong stretching
1055.84	1054.87		C–O strong stretching
1031.73	1031.73	1031.73	C–O strong stretching
957.484			Isoindol deformation
917.95	917.95		Isoindol deformation
862.025	868.774	865.882	C–H bending
826.348	826.348	826.348	C–H bending
	803.206		C–H bending
788.743	789.707	789.707	C–H bending
748.245	748.245	748.245	C–H bending
647.965	647.001	647.965	C–H bending
576.612	576.612	575.647	C–H bending
545.756	545.756	545.756	Stretching Al–O vibration
504.294	503.33		Stretching Al–O vibration
455.118	458.011	460.904	Stretching Al–O vibration
419.442	418.477	418.477	Stretching Al–N vibration

from a quartz crucible source heated by a tungsten coil in a vacuum of 10^{-4} Pa. The film was deposited onto pre-cleaned glass substrate (for structure investigation) and diffused optically flat quartz substrates (for optical investigation). The thickness of the films was determined using a quartz crystal thickness monitor (Edwards, Model FTM4) and calibrated by Tolansky's technique [13]. The as-deposited Alq_3 thin film was annealed at 473 K for 2 h under vacuum of 10^{-1} Pa. A Philips X-ray diffractometer (model X' pert) was used for the measurements of structural properties with utilized monochromatic Cu K_α radiation ($\lambda = 1.5418$ Å) operated at 40 kV and 25 mA. Fourier Transformation Infrared transmission (FTIR) spectra for the powder, the as-deposited and annealed thin films of Alq_3 were studied to confirm the molecular structure of Alq_3 compound. The measurements were performed using (Buker, Vector 22) infrared spectrophotometer in the range 400–2000 cm^{-1}. The morphology of the as-deposited and annealed Alq_3 thin films were studied using transmission electron microscope (TEM) of type (JEOL JEM-1230).

Optical properties were investigated for the as deposited and annealed thin films by spectrophotometric measurements of transmittance, T, and reflectance, R, at normal incidence in the spectral range from 200 to 2500 nm, using a double-beam spectrophotometer (JASCO model V-570 UV–vis–NIR) attached to a specular reflection stage.

2.2. Optical properties

The absolute values of the measured transmittance, T, and reflectance, R, after correction of the absorbance and reflectance of the substrate are given by [14,15]

$$T = \left(\frac{I_{ft}}{I_q}\right)(1 - R_q) \tag{1}$$

where R_q is the reflectance of quartz. I_{ft} and I_q are the intensities of light passing through – quartz system and reference quartz substrate, respectively, and

$$R = \left\{\left(\frac{I_{fr}}{I_m}\right) R_m(1 + [1 - R_q]^2)\right\} - T^2 R_q \tag{2}$$

where I_{fr} and I_m are the intensities of light reflected from the sample and that from reference mirror, respectively, R_m is the reflectance of Al-mirror and R_q is the reflectance of quartz.

The refractive index (n) and the extinction coefficient (k) of the thin films at different wavelengths can be calculated by using the following equations:

$$\alpha = \left(\frac{1}{d}\right) \ln\left[\frac{(1-R)^2}{2T} + \sqrt{\frac{(1-R)^4}{4T^2} + R^2}\right] \tag{3}$$

$$n = \frac{1+R}{1-R} + \sqrt{\frac{4R}{(1-R)^2} - k^2} \tag{4}$$

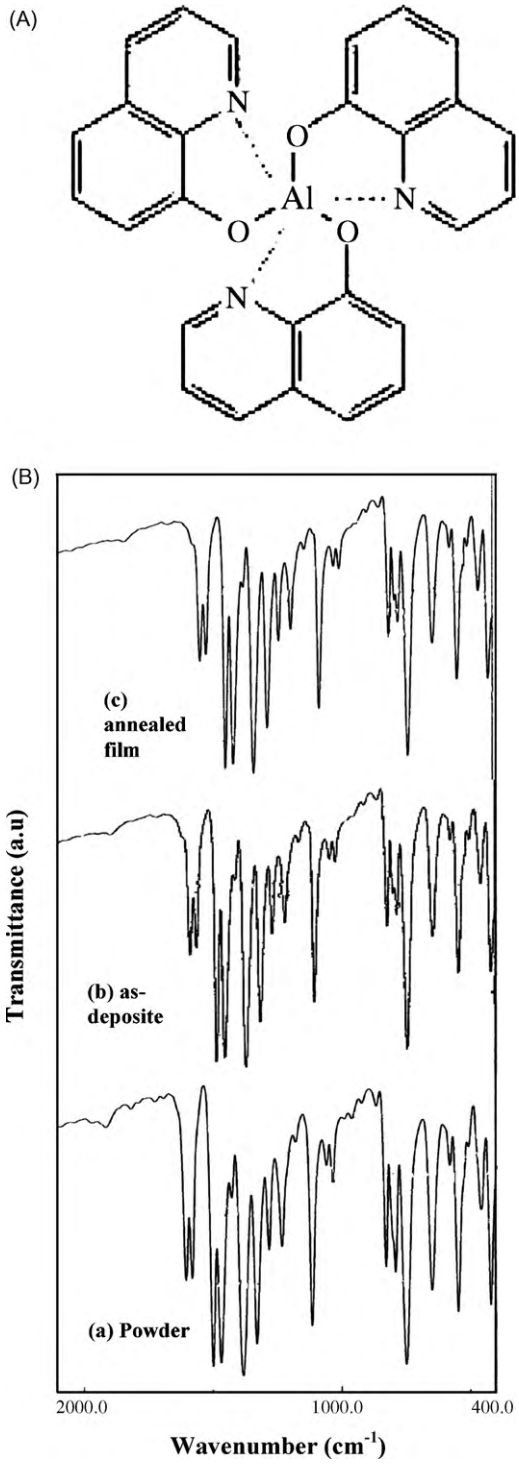

Fig. 1. (A) The chemical configuration of $Alq_3(C_{27}H_{18}AlN_3O_3)$. (B) The infrared spectra of Alq_3 in powder form, as-deposited and annealed (at 473 K for 2 h) thin films.

$$k = \left(\frac{\alpha\lambda}{4\pi}\right)$$

where α is the absorption coefficient and d is the film thickness.

By knowing (d), unique values of (n) and (k) can be obtained. The experimental errors were taken into account as ±5% for the film thickness measurements and ±1% for T and R. The error in the calculated values of n and k were estimated to be ±3% and 2.5%, respectively.