The Optical Band Gap based on K-M Function on Layer of LiTaO3 with Variation Treatment of Annealing Temperature

by Nani Djohan

The Optical Band Gap based on K-M Function on Layer of $LiTaO_3$ with Variation Treatment of Annealing Temperature

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***Abstract*—The thin layer made from the material of $LiTaO_3$ on a P-type silicon wafer has been produced by using Chemical Solution Deposition (CSD) technique. In this study, the thin films have been annealed with thermal differences in the furnace (Nabertherm B410) for 15 hours at a temperature of 750°C, 800°C, and 850°C. The reflectance data which are related with the characteristic of thin films have been measured by using deuterium-halogen light sources (Ocean Optics DH-2000-BAL) and spectrometer (Ocean Optics USB4000-UV-VIS) in the wavelength range of 230-850 nm. The K-M (Kubelka-Munk) function is applied to estimate the optical band gap value that is referred to the reflectance data and photon energy. The result of this study shows that the optical band gap of $LiTaO_3$ material on P-type silicon wafers are having a shift of sensitivity in accordance with the increment of temperature. Based on the result of optical band gap values which are related to light spectrum, it is concluded that the thin films have the sensitivity in the ultraviolet, visible, and near-infrared region.**

Keywords*—*$LiTaO_3$, CSD, temperature, K-M function, optical band gap

I. Introduction

Atom is the smallest fraction of an element which is structured from proton, neutron, and electron [1]. In the crystalline structure, the atoms or groups of atoms are uniquely composed in a three-dimensional pattern that is very ordered [2, 3]. The smallest repeating pattern that represents the atomic lattice in the crystalline structure is called a unit cell [2]. According to the experimental study of optical materials, the presence of light can leads to a number of phenomena refering to the recombination process of electron-hole pairs (motion of electrons) in the lattice [4].

The optical properties of materials can be characterized from the interaction with visible light particles or electromagnetic radiation (called photons) [5, 6, 7]. More importantly, the interaction of photons in the crystalline structure of a material can affect the motion of electrons which are capable of generating a number of phenomena related to absorption, refraction, and transmission intensities [5, 7]. In addition, the classification of a group of materials (metal, insulator, and semiconductor) can be determined from the behavior of electrons (excitation and transfer) based on band gap which is expressed in terms of electron volts (eV) [8, 9, 10].

Absorbance, reflectance, and transmittance are the basic measurements that are used for investigating the properties of materials regarding the interaction of photons on the surface area [5, 7, 11]. In this study, the spectral of reflectance from the fabrication of thin films ($LiTaO_3$ on the surface of P-type silicon wafers) are measured by using spectrometer with deuterium-halogen light sources in the regions of 230-850 nm. Furthermore, the K-M (Kubelka-Munk) function is used to estimate the band gap value and identify the sensitivity of light spectrum of a thin film by utilizes the reflectance data (spectral reflectance) [12-17].

II. Methodology

The preparation was begun by shaping the piece of a silicon wafer with the area of 1 × 1 cm², then cleaned sequentially using acetone (C_3H_6O), methanol (CH_3OH), and deionized water during 15 minutes in an ultrasonic tub. Moreover, the silicon wafers were dried at room temperature. In this study, the molecular formula of lithium tantalate ($LiTaO_3$) was obtained from the synthesis of lithium acetate ($C_2H_3LiO_2$) and tantalum (v) methoxide ($Ta(OCH_3)_5$) in accordance with the balance of chemical equation:

$$2C_2H_3LiO_2 + 2Ta(OCH_3)_5 + 19O_2 \rightarrow 2LiTaO_3 + 14CO_2 + \ldots \\ \ldots + 18H_2O \quad (1)$$

According to (1) and the molarity of chemical reaction which is organized at 1 M, composite of the mass of $C_2H_3LiO_2$ (0.16496 g) and $Ta(OCH_3)_5$ (0.84030 g) were dissolved in 2.5 ml of 2-methoxyethanol, accompanied with homogenizing the chemical solution for 90 minutes by using an ultrasonic device. For the further summary, Fig. 1 shows the sequential schematic that occurs in this methodology related to fabrication and measurement of thin films that made from the layer of $LiTaO_3$ on the surface of P-type silicon wafer.

Based on Fig. 1, the coating process of $LiTaO_3$ on a silicon wafer (see Fig. 2) was done by referring to the Chemical Solution Deposition (CSD) technique, i.e. dripping the solution on the surface of a silicon wafer and spinning it on the rotating disc (spin coater device) at speed of 4000 rpm for 30 seconds. The fabrication of thin films was terminated by heating the $LiTaO_3$ material on a P-type silicon wafer in the furnace (Nabertherm B410) at a temperature of 750°C, 800°C, and 850°C for 15 hours [18, 19, 20].

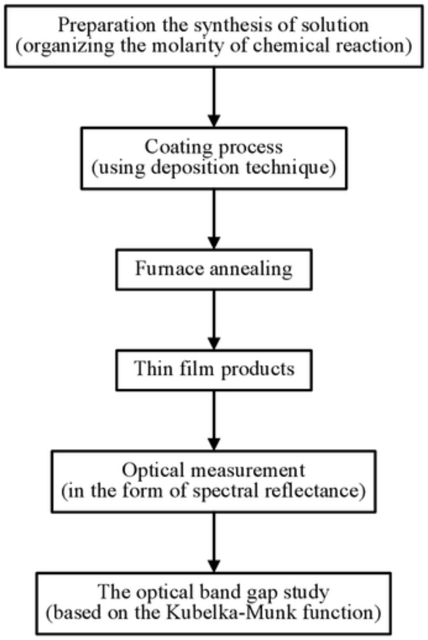


Fig. 1. Schematic of methodology

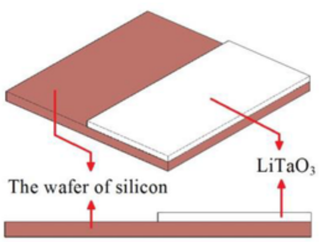


Fig. 2. $LiTaO_3$ on the silicon wafer

To support of this study, the devices of deuterium-halogen light sources (Ocean Optics DH-2000-BAL) and spectrometer (Ocean Optics USB4000-UV-VIS) were specifically used to measure the optical characterization of thin films in the form of spectral reflectance with the wavelength range of 230-850 nm. Based on this measurement, the Kubelka-Munk function was utilized to estimate the optical band gap on each thin film that has been fabricated in this study.

III. Result and Discussion

In this study, the measurement of thin films was displayed in the form of spectral reflectance (Reflectance (%)) as a function of the wavelength of light (see Fig. 3). Based on Fig. 3, the optical band gap of thin films was described in the coordinate axis by referring to the formula:

$$F(R) = \frac{(1-R)^2}{2R} \tag{2}$$

$$x\text{-}axis = hv \tag{3}$$

$$y\text{-}axis = (F(R)\ hv)^n \tag{4}$$

with:
R = reflectance value (in the regions of 230-850 nm)
F(R) = the Kubelka-Munk function
hv = the energy of photon (eV)
n = 2 for allowed direct transition
n = 0.5 for allowed indirect transition

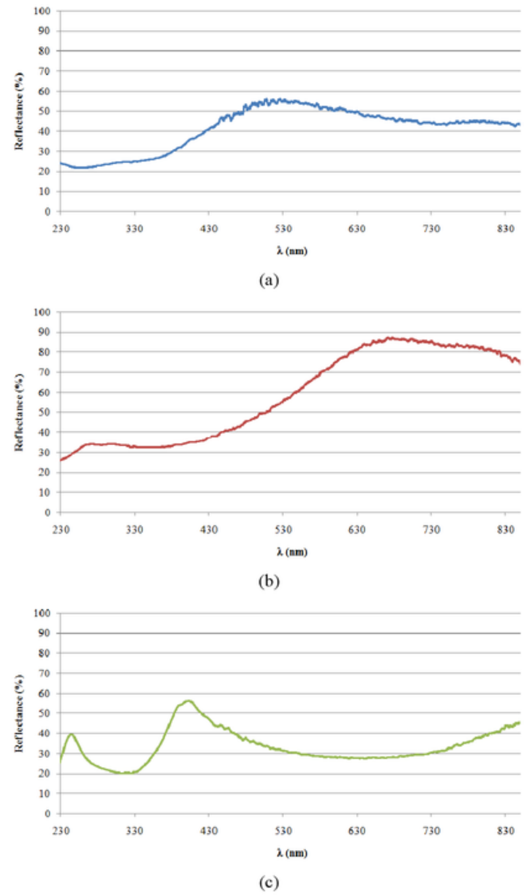
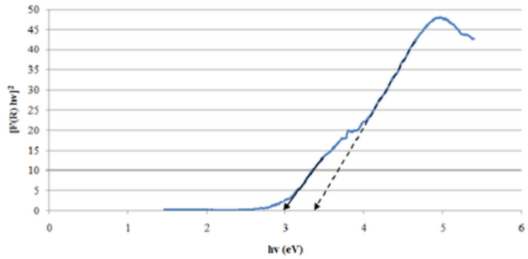


Fig. 3. Spectral of light reflectance: (a) 750°C (b) 800°C (c) 850°C

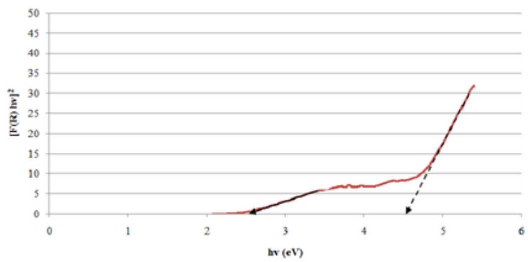
Related to the previous study, the Tauc plot method was used to extrapolation the optical band gap value of this thin films (listed in TABLE I) through a withdrawing straight line from $(F(R)\ hv)^n$ to hv (see Fig. 4). Moreover, the wavelength of each thin film can be discovered through the calculation (listed in TABLE II) using the following formula:

$$\lambda = \frac{hc}{(1.602 \times 10^{-19}\ J)(the\ optical\ band\ gap)} \tag{5}$$

with:
h = Planck's constant (6.626×10^{-34} J·s)
c = speed of light (2.998×10^{8} m·s^{-1})
the optical band gap = from listed in TABLE I



(a)



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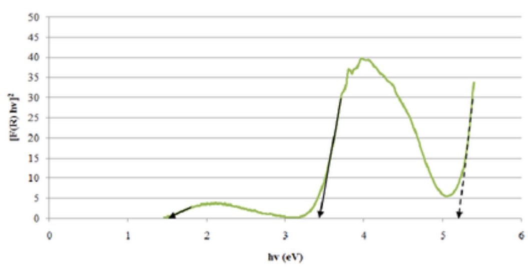

(c)

Fig. 4. Extrapolation of the optical band gap: (a) 750°C (b) 800°C (c) 850°C

TABLE I. THE OPTICAL BAND GAP OF THIN FILM

Annealing Temperature (°C)	Optical Band Gap (eV)
750	2.97
	3.38
800	2.53
	4.53
850	1.52
	3.43
	5.21

TABLE II. THE WAVELENGTH AND CLASSIFICATION OF LIGHT SPECTRUM OF EACH THIN FILM

Annealing Temperature (°C)	Wavelength of Light (nm)	Classification of Light Spectrum
750	418	Visible
	367	Ultraviolet
800	490	Visible
	274	Ultraviolet
850	816	Infrared
	362	Ultraviolet
	238	

IV. CONCLUSION

In this fabrication, the Chemical Solution Deposition (CSD) technique and annealing process have been applied to form the thin layer of $LiTaO_3$ on the surface of P-type silicon wafer. Furthermore, the optical response of the thin layer is identified based on the measurement in the form spectral of light reflectance in the wavelength range of 230-850 nm, then it is investigated by using the Kubelka-Munk function to obtain the optical band gap values. Based on the result of this study, it is concluded that the thin films have the sensitivity in the ultraviolet, visible, and near-infrared region.

ACKNOWLEDGMENT

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