The optical band gap of LiTaO3 and Nb2O5-doped LiTaO3 thin films based on Tauc Plot method to be applied on satellite

by Richie Estrada

IOP Conference Series: Earth and Environmental Science

PAPER • **OPEN ACCESS**

The optical band gap of $LiTaO_3$ and Nb_2O_5-doped $LiTaO_3$ thin films based on Tauc Plot method to be applied on satellite

To cite this article: R Estrada *et al* 2017 *IOP Conf. Ser.: Earth Environ. Sci.* **54** 012092

The optical band gap of $LiTaO_3$ and Nb_2O_5-doped $LiTaO_3$ thin films based on Tauc Plot method to be applied on satellite

R Estrada[1*], N Djohan[1], D Pasole[2], M Dahrul[3], A Kurniawan[3], J Iskandar[3], H Hardhienata[4] and Irzaman[4]

[1] Department of Electrical Engineering, Faculty of Engineering and Computer Science, Krida Wacana Christian University, Jl. Tj. Duren Raya No. 4, Jakarta 11470, Indonesia.

[2] Student of Electrical Engineering, Faculty of Engineering and Computer Science, Krida Wacana Christian University, Jl. Tj. Duren Raya No. 4, Jakarta 11470, Indonesia.

[3] Post Graduate of Biophysics, Faculty of Mathematics and Natural Sciences, Bogor Agricultural University, Jl. Raya Dramaga, Bogor 16680, Indonesia.

[4] Department of Physics, Faculty of Mathematics and Natural Sciences, Bogor Agricultural University, Jl. Raya Dramaga, Bogor 16680, Indonesia.

E-mail: richie.estrada@ukrida.ac.id

Abstract. This research observed the optical band gap of thin films made from $LiTaO_3$ undoped (0%) and doped (5% and 10%) with Nb_2O_5 in the 1 M-solubility deposited on n-type Si (111) substrates. The thin films are manufactured with coating process of substrates by Chemical Solution Deposition (CSD) method using a spin coater device at a rotation speed of 3000 rpm for 30 seconds and annealed in furnace (Nabertherm B180) at a temperature of 850°C for 15 hours. The optical absorption data of thin films are obtained by using an Ocean Optics USB2000 device in the wavelength of visible light. The band gap curve is determined from optical absorption data processing using Tauc Plot method. The Tauc Plot with indirect transition shows that $LiTaO_3$ doped with Nb_2O_5 provides increased optical band gap value in a range less than 3.5 eV. Based on the results of this research, it can be concluded that $LiTaO_3$ and Nb_2O_5-doped $LiTaO_3$ thin films on n-type Si (111) substrate are semiconductor materials and has the potential to be applied on satellite.

1. Introduction

Thin film is a layer of material with the thickness of 10^{-9} m – 10^{-6} m that is grown by using the surface of substrate [1, 2]. The layer of material can be made of organic, inorganic, metal and organometallic which contain conductor, semiconductor, superconductor and insulator properties [3-6]. Basically, atomic structure in the material is divided into two (2) groups of energy band. The band with lower energy is called valence band, whilst the other with higher energy is called conduction band. The area between valence band and conduction band is separated by forbidden band. The amount of energy required to discharge electrons from valence band to conduction band is called the 'band gap' (unit: eV) [7, 8].

The crystal structure in the form of chemical formula ABO_3 is called perovskite [9, 10]. Lithium tantalate ($LiTaO_3$) is an inorganic material [11] that has 4.7 eV of band gap [12] and one of alkali tantalate type perovskite family rhombohedral crystal structure with space group of R3c [13-15] (see Figure 1). Previous studies argued that the doping concentration could change crystalline structure of perovskite [16, 17] that affected the shifts in band gap [1, 18, 19]. Thus, the focus of this research is to investigate the optical band gap of $LiTaO_3$ and Nb_2O_5-doped $LiTaO_3$ thin films on n-type Si (111) substrates using Tauc Plot method from UV-Vis Ocean Optics USB2000 as the measurement device.

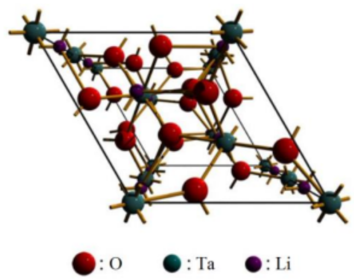


Figure 1. Crystal structure of $LiTaO_3$ [10]

2. Methodology

Lithium tantalate ($LiTaO_3$) was obtained from the result of mixing chemicals powder between lithium acetate ($Li(CH_3COO)$) and tantalum pentoxide (Ta_2O_5) according to balanced chemical equation [18]:

$$2Li(CH_3COO) + Ta_2O_5 + 4O_2 \rightarrow 2LiTaO_3 + 4CO_2 + 3H_2O \quad (1)$$

The solubility of this research was regulated at 1 M to calculate mass composition from lithium acetate powder ($Li(CH_3COO)$, 99.5% purity) and tantalum pentoxide powder (Ta_2O_5, 99.9% purity) corresponding with balanced chemical equation. The result of mass composition calculation indicates the exact amount of lithium acetate powder ($Li(CH_3COO)$, 99.5% purity) is 0.1650 gram and tantalum pentoxide powder (Ta_2O_5, 99.9% purity) is 0.5524 gram. In this research, the niobium oxide powder (Nb_2O_5, 99.9% purity) was used as a doping for lithium tantalate ($LiTaO_3$) with a mass composition of 0.0295 gram (5% from the mass of $LiTaO_3$) and 0.0590 gram (10% from the mass of $LiTaO_3$). The entire calculation of mass composition from chemicals powder (lithium acetate, tantalum pentoxide and niobium oxide) was weighed using analytical scale (AND GR-200).

A thin layer in form of liquid was made by mixing the chemicals powder into the solvent 2-methoxyethanol ($CH_3OCH_2CH_2OH$) with 2.5 ml volume to produce solution formulations of $LiTaO_3$, $LiTaO_3$ + 5% Nb_2O_5 and $LiTaO_3$ + 10% Nb_2O_5. All solution formulation was sonicated by using ultrasonicator device (BRANSON 2510) for 90 minutes to obtain the homogeneous solutions. The coating process of each homogeneous solutions on a n-type Si (111) substrates (half surface from dimensions of 1×1 cm^2) were done with Chemical Solution Deposition (CSD) method using a spin coater device at speed of 3000 rpm for 30 seconds [20]. Each coating process (dripping and rotating) was repeated three (3) times with interruption time for one (1) minute, then annealed in furnace (Nabertherm B180) at a temperature of 850°C for 15 hours.

Research on this thin films referred to the measurement of absorption spectra (optical characterization) from a thin layer that was formed on n-type Si (111) substrates. UV-Vis spectroscopy (Ocean Optics USB2000) was used as a device to measure the absorption spectra (optical characterization) on thin films in the form of absorbance value at a wavelength of visible light. Absorbance value indicates the magnitude of photon energy absorbed by a thin layer due to the influence of excitation of electrons from valence band to conduction band. The optical band gap value for each thin film was determined through extrapolation by withdrawing straight line on curve that was formed from correlation between $(\alpha h\nu)^n$ and $h\nu$ (called Tauc Plot method).

3. Result and Discussion

In this research, the measurement of optical absorbance from thin layer that deposited on n-type Si (111) substrate was presented in absorption spectra (see Figure 2). Related to optical absorbance, the coordinate axes for optical band gap of thin films were determined from the calculation using the following formula (equation) [1, 21, 22]:

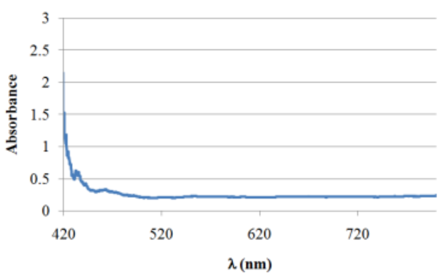
$$d = \frac{m}{\rho A} \quad (2)$$

$$\alpha = 2.303 \frac{\text{optical absorbance}}{d} \quad (3)$$

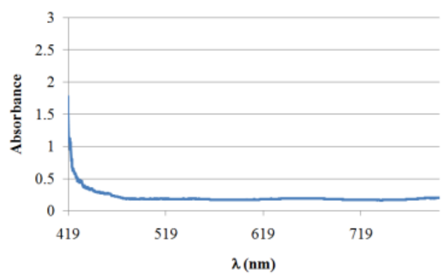
$$\text{y-axis} = (\alpha h\nu)^{0.5} \quad (4)$$

$$\text{x-axis} = h\nu \quad (5)$$

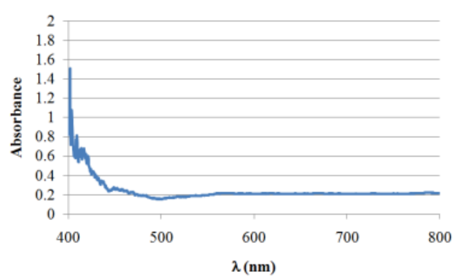
with: m = mass of thin layer on n-type Si (111) substrate (gram)
ρ = density of $LiTaO_3$ (7.46 gram/cm^3)
A = surface area of thin layer on n-type Si (111) substrate (cm^2)
d = thickness of thin layer on n-type Si (111) substrate (cm)
optical absorbance = data values (from measurement using an Ocean Optics USB2000)
α = absorption coefficient (cm^{-1})
$h\nu$ = photon energy (eV)



(a)



(b)



(c)

Figure 2. Absorption spectra: (a) Undoped (b) Doped with 5% Nb_2O_5 (c) Doped with 10% Nb_2O_5

The Tauc Plot for undoped and Nb_2O_5-doped $LiTaO_3$ thin films on n-type Si (111) substrate were presented in Figure 3. The band gap values were determined through extrapolation by withdrawing straight line (as shown in Figure 3) on coordinate axes ($(\alpha h\nu)^{0.5}$ – $h\nu$) and listed in Table 1. The wavelengths of thin films were obtained from the calculation (listed in Table 2) using the following formula (equation) [1]:

$$\lambda = \frac{h\,c}{\left(1.602 \times 10^{-19}\ \mathrm{J}\right)\left(\text{optical band gap}\right)} \tag{6}$$

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

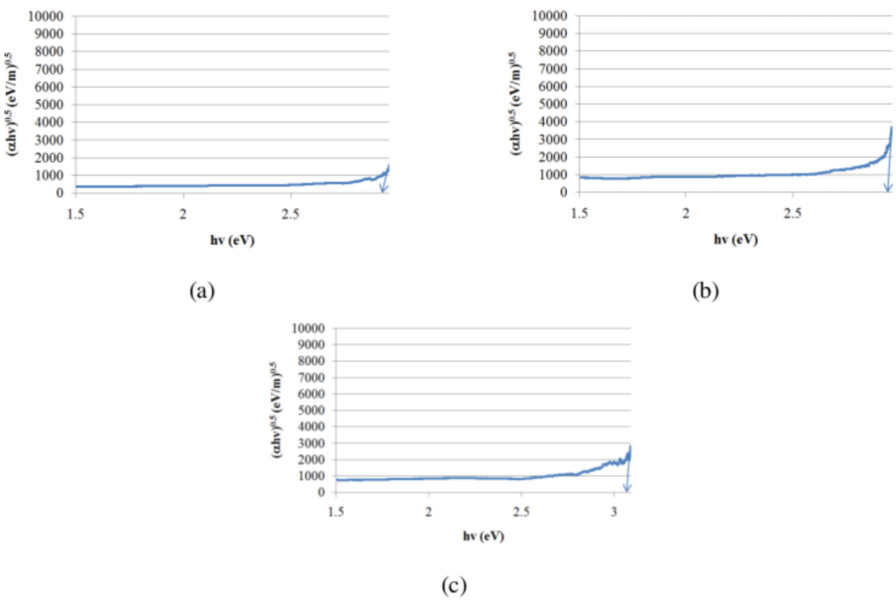


Figure 3. Optical band gap: (a) Undoped (b) Doped with 5% Nb_2O_5 (c) Doped with 10% Nb_2O_5

Table 1. The optical band gap of thin films

	Optical band gap (eV)
$LiTaO_3$ + 0% Nb_2O_5	2.93
$LiTaO_3$ + 5% Nb_2O_5	2.95
$LiTaO_3$ + 10% Nb_2O_5	3.07

Table 2. The wavelength and sensitivity to specific spectra color of light on each thin film

	Wavelength of light (nm)	Spectra color of light (Based on literature [23])
$LiTaO_3$ + 0% Nb_2O_5	424	Violet
$LiTaO_3$ + 5% Nb_2O_5	421	Violet
$LiTaO_3$ + 10% Nb_2O_5	404	Violet

4. Conclusion

In this research, the thin film shows increasing optical band gap values through the addition of Nb_2O_5 (5% and 10%) into $LiTaO_3$. Based on the optical band gap values of this research, it can be concluded that the grown of $LiTaO_3$ and Nb_2O_5-doped $LiTaO_3$ thin films on n-type Si (111) substrate are classified into semiconductor materials and has the potential to be applied on satellite.

Acknowledgment
This research is funded by the Ministry of Research, Technology and Higher Education of the Republic of Indonesia through PEKERTI Research Grant No. 771/K3/KM/SPK.LT/2016.

References

[1] Ohring M 1992 *The Materials Science of Thin Films* (San Diego: Academic Press)
[2] Hong X, Gan Y and Wang Y 2011 *Surf. Interface Anal.* **43** 1299
[3] Mercereau J E and Notarys H A 1973 *J. Vac. Sci. Technol.* **10** 646
[4] Fraxedas J 2008 *Molecular Organic Materials: From Molecules to Crystalline Solids* (Cambridge: Cambridge University Press)
[5] Schlueter J A 2009 *Top. Organomet. Chem.* **27** 1
[6] Wang X L, Dou S X and Zhang C 2010 *NPG Asia Mater.* **2** 31
[7] Shur M 2005 *The Electrical Engineering Handbook* ed W K Chen (San Diego: Academic Press) p 153
[8] Wang W, Tadé M O and Shao Z 2015 *Chem. Soc. Rev.* **44** 5371
[9] Inaguma Y, Matsui Y, Shan Y J, Itoh M and Nakamura T 1995 *Solid State Ionics* **79** 91
[10] Su Y, Lang J, Du C and Wang X 2016 *Perovskite Materials - Synthesis, Characterisation, Properties, and Applications* ed L Pan and G Zhu (Rijeka: InTech) **Chapter 16** pp 489–510
[11] Brehmer L, Kaminorz Y, Dietel R, Grasnick G and Herkner G 1997 *Frontiers in Biosensorics I: Fundamental Aspects* ed F W Scheller, F Schubert and J Fedrowitz (Basel: Birkhäuser Verlag) pp 155–166
[12] Nuraje N, Kudaibergenov S and Asmatulu R 2013 *Producing Fuels and Fine Chemicals from Biomass Using Nanomaterials* ed R Luque and A M Balu (Boca Raton: CRC Press) **Chapter 4** pp 95–118
[13] Tarafder A, Annapurna K, Chaliha R S, Tiwari V S, Gupta P K and Karmakar B 2010 *J. Alloy. Compd.* **489** 281
[14] Khalil A, Masaif N, Jennane A and Maaider K 2011 *J. Mater. Environ. Sci.* **2** 196
[15] Tahiri M, Masaif N, Jennane A and Lotfi E M 2012 *Ukr. J. Phys.* **57** 834
[16] Shen K, Sun H L, Ji G, Yang Y, Jiang Z and Song F 2016 *Nanoelectronics and Materials Development* ed A Kar (Rijeka: InTech) **Chapter 6** pp 95–116
[17] Zhang T, Dong Y T, Geng T, Dai Q and Xu Y H 2009 *J. Mater. Chem. Phys.* **114** 257
[18] Rundupadang G C, Estrada R, Kurniawan A, Rohaeti E dan Irzaman 2015 *Prosiding Seminar Nasional Fisika dan Aplikasinya (Jatinangor)* **1** (Sumedang: Universitas Padjadjaran) p FM-07
[19] Irzaman, Pebriyanto Y, Apipah E R, Noor I and Alkadri A 2015 *Integrated Ferroelectrics* **167** 137
[20] Estrada R, Djohan N, Rundupadang G C, Kurniawan A, Iskandar J, Dahrul M, Hardhienata H and Irzaman 2016 *presented in 2nd Int. Conf. on Sci. Tech. and Interdiscip. Res. 2016 (Lampung)* (Bandar Lampung: University of Lampung) [Unpublished]
[21] Ismangil A, Jenie R P, Irmansyah and Irzaman 2015 *J. Procedia Environ. Sci.* **24** 329
[22] Triloki, Rai R and Singh B K 2013 *Proc. Int. Symp. on Nuclear Phys. (Mumbai)* **58** (India: Bhabha Atomic Research Centre) p 838
[23] Bharadwaj V 2014 *Proc. Natl. Conf. Comp. of Colours (Indore)* (Madhya Pradesh: Granthaalayah) pp 1–6

The optical band gap of LiTaO3 and Nb2O5-doped LiTaO3 thin films based on Tauc Plot method to be applied on satellite

ORIGINALITY REPORT

16%	15%	6%	2%
SIMILARITY INDEX	INTERNET SOURCES	PUBLICATIONS	STUDENT PAPERS

PRIMARY SOURCES

1	www.arpnjournals.org Internet Source	6%
2	id.123dok.com Internet Source	2%
3	www.ijert.org Internet Source	1%
4	epdf.pub Internet Source	1%
5	Submitted to Boston University Student Paper	1%
6	www.yumpu.com Internet Source	1%
7	Pravin Jagadale, Maheshwar Sharon, Madhuri Sharon, Golap Kalita. "Carbon Thin Films from Plant-Derived Precursors", Synthesis and Reactivity in Inorganic, Metal-Organic, and Nano-Metal Chemistry, 2007 Publication	1%

8	journals.iucr.org Internet Source	1 %
9	repository.lppm.unila.ac.id Internet Source	1 %
10	www.hindawi.com Internet Source	1 %

Exclude quotes	Off	Exclude matches	< 1%
Exclude bibliography	On		