

Simulation Analysis of Optical Properties of Indium Tin Oxide

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Abstract

TCO (transparent conduction oxides) have been suitable materials for optoelectronics applications, Indium Tin Oxide is an n-type transparent conducting oxide semi-conductor, which possess a combine property of transparency to visible light and electrical conductivity, its features have been studied in this paper using MATLAB computer programming. The features which consist optical and electrical properties were simulated using MATLAB programming, the drive ITO models were used within the range and limit of other researchers, whose have done the researches experimentally. The models were used to simulate optical transmittance, optical absorptions, and reflectance of ITO, which all depends on films thicknesses.

Keywords: *Transparent Conducting Oxide; Indium Tin Oxide; Reflectance; Matlab; Thickness.*

1. Introduction

ITO (Indium Tin Oxide) was first reported by G. Rupprecht in 1954. Among the class of TCO (Transparent Conducting Oxide) film, ITO due to its technologically important, has been widely used which has combination of properties such as high visible light range transmittance, low electrical resistivity, high infrared reflectance, excellent substrate adherence, chemical inertness and hardness (Lam, 2014).

ITO having a low electrical resistivity and high free carrier density is considered to be a wide band gap material. Indium tin oxide have been widely used as transparent conducting oxide in solar cells, touch screen, light emitting diodes (LEDs), sensors, liquid crystal displays and smart window (Taha et al., 2018). As a result of its low electrical resistivity of about $2-4 \times 10^{-4} \Omega \text{ cm}$, It is known to be an n-type semiconductor (Kim et al., 1999). It was reported that, ITO materials has direct wide band gap energy between 3.5 - 4.3 eV (Chen et al., 2013). The transparency to visible light ($\text{In}_2\text{O}_3:\text{SnO}_2$) has been attribute to its band gap energy, while its conductivity originates from its intrinsic oxygen vacancies and extrinsic Sn⁴ doping In³ atoms are replaced with Sn to form cubic bixbyite structure of indium oxide. Lam, 2014 suggested that, each cation rest at the center of the cube while the oxygen anions are positioned at the six corners (Lam, 2014)

It is also reported that heavy doping in ITO lead to large carrier concentration, thus ITO materials are a highly degenerated semiconductors (Meng, et.al, 2008). Another research revealed that, Increase in impurity concentrations result in decrease in the distance between the impurities atoms, as the increment is sustained a point is reached when this donor electrons will start to interact with each other (Mohamed et al., 2009). Furthermore, to widen the band of the donor state, increase in donor concentration is required and subsequently may even overlap the bottom states of the conduction band. Hence, The fermi level (E_F) will now be shifted to the conduction band (Benama et.al, 1999). As the donor concentration become comparable with the resulting density of electronic state, overlapping take place. As E_F moves to the higher energy level within the conduction band, the minimum electronic state closer to the conduction band are completely occupied. Therefore, higher energy is required to excite electrons from the valence band to those available electronic state in the conduction



band (Kaushik et al., 2017). Hence, as the concentration increases, the effective band gap of the indium tin oxide increases (Benamar et al., 1999).

1.1 Application in Optoelectronics

ITO has been used as a transparent contact in advanced optoelectronic devices such as solar cells, light emitting and photo diodes, photo transistors and lasers - some for the first time as a result of this investigation (Afre, Sharma, Sharon, & Sharon, 2018). Zinc Oxide (ZnO) and Fluorine Tin oxide (FTO), and Gallium-doped Tin Oxide (GITO) are TCO thin film material that have been used for the above listed application of TCO (Akinkuade et al., 2018 and Shirakata et al., 2003) .ITO is the most widely used due to its electrical conductivity and high optical transmittance in the visible region of light spectrum (Isiyaku et al., 2019). Thus it is soon becoming an integral part of modern electronic technology wherever there is a potential for improving optical sensitivity of light detecting devices or quantum efficiency of light emitting devices (Schultz et al., 2017).

2. Materials and Methodologies

A model of ITO as a function of Optoelectronics was formulated to investigate the optical behavior of ITO on reflectance dependence, optical absorption and transmittance.

2.1 Model Equations

ITO Optical Transmittance T depends on optical thickness topt which is written as

$$t_{opt} = (m + 1) \frac{\lambda}{4n} \tag{1}$$

where m is either 0 or an even integer.

λ is the wavelength.

n is the refractive index, which is 1.96.

Similarly, transmission coefficient is given by

$$T = \exp(-\alpha t) \tag{2}$$

Where α is the optical absorption

Hence, equation 2 can be rewriting as

$$T = \exp(-\alpha(m + 1) \frac{\lambda}{4n}) \tag{3}$$

Thus, reflectance dependence coefficient is given by

$$R + T = 1 \tag{4}$$

Also

$$R = 1 - \frac{1}{\alpha t} \exp t \tag{5}$$

$$t = (m + 1) \frac{\lambda}{4n}$$

From

$$T = (1 - R) \exp(-\alpha t) \tag{6}$$

The two importance parameters that simulate optimization electrical conductivity and optical transmission of transmittance conducting films are thickness t and sheet resistance R_s .

$$R_s = \frac{\rho}{t} = \frac{1}{\sigma t} \tag{7}$$

From equation 2 and 7 Optical transmittance and wavelength dependent coefficient will be written as

$$\alpha = \frac{4}{(m+1)\lambda} \ln\left(\frac{1}{T}\right) \tag{8}$$

From the above equations, it is clear that optoelectronics properties depend on thickness of the films, reflectance and transmission. MATLAB program was used to plot and simulate the above parameters. Result obtained was in agreement with the experimental and theoretical work available in the literature.

Optical absorption coefficient from range of 0 to 0.020, and wavelength from range of 0 to 1300 nm are selected after a careful consideration of the material feature from the work of (Cui et al., 2002 and Isiyaku et al., 2017).

3. Results

As most of research are concentrated in enhancing Indium Tin Oxide (ITO) optical properties, in this work we focus on improved method of determining the optical and electrical properties of ITO (Kerkache & Layadi, 2005). Wavelength dependent Transmission and Reflectance coefficients were obtained by equation (3 and 4) above. Furthermore, the reflectance decreases with the increase of film thickness in the visible range of wavelength 400nm to 700nm this is in agreement with the experimental work (Kamarudin et.al, 2014) (Salehi, 1998) the three curves represent ITO reflectance at three values of m , m could be 0 or even integers. The actual film thickness of 2063, 3437, 4812 nm (corresponding to $3\lambda/4$, $5\lambda/4$ and $7\lambda/4$ optical thickness respectively) this is in agreement with the experimental work (State & Road, 1981). The Fig 1 below present simulated results, which Fig 2 is a work of (Kamarudin et al., 2014) for comparison.

In the fig below the reflectance as a function of wavelength is presented. Fig 1 is for simulated result, while Fig 2 is a experimental result from for comparison.

It can be observed that the optical reflectance decreases with the increasing film thicknesses. Similarly, large ITO films thickness brought about high scattering effects whereas the low thickness reduces the optical scattering effect. This reflectance thickness phenomena was similarly highlighted in the experimental works of Kamarudin et al. (2014) and Salehi (1998) respectively.

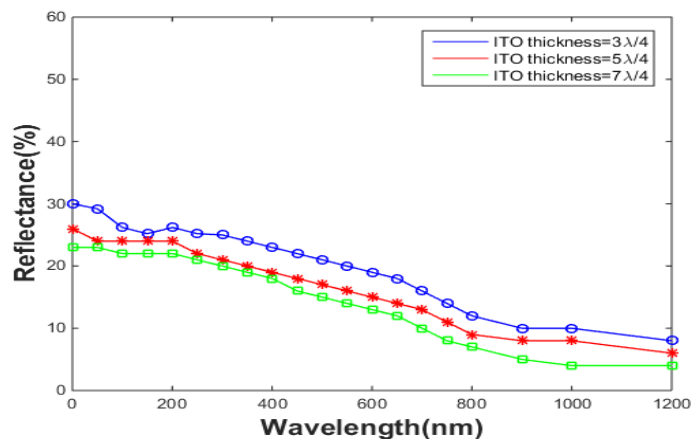


Figure 1: Simulated ITO films reflectance with respect to films thickness of the film few layers of ITO films.

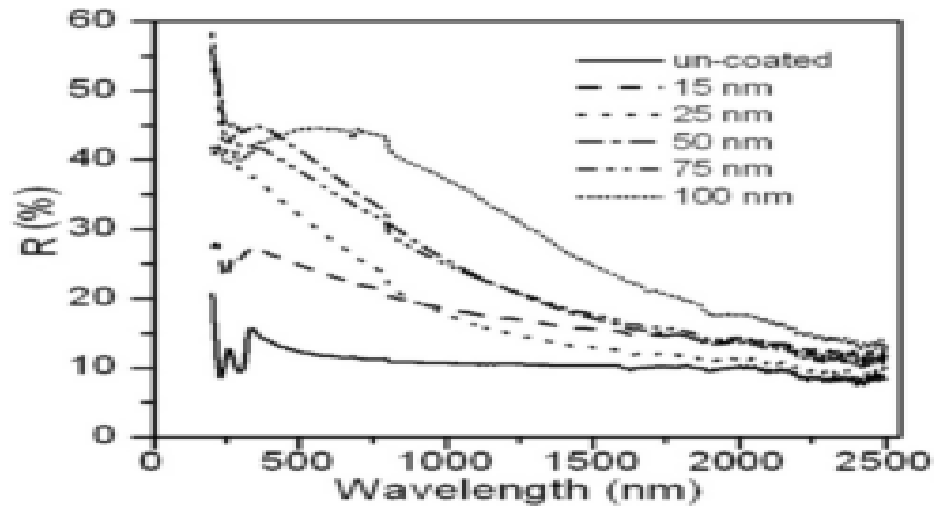


Figure 2: experimental of Kamarudin et al. (2014). ITO films reflectance with respect to films thickness of the film few layers of ITO films, for comparison with simulation result

TCO have high transmission abilities as well as low resistivity for use in solar cells. Fig. 3 presents the trend of transmission of ITO film thickness. High transmission is obtained for very thin ITO thickness while larger films thickness reveals low optical transmission as also indicated in the work of (Kim & Gilmore, 1999).

High transmission of about 91 % in the visible region was obtained for film with lowest thickness whereas the film with largest film exhibits about 85 % in the same region revealing a low optical transmission. For a good ITO films, high transmittance and good electrical conductivity properties are obtained (Isiyaku et al., 2019). Furthermore, the trend of optical transmittance (Figure 3 and 4) for the simulated and experimental works are in good agreement. The results also harmonized with the works of (Alsultany et al, 2014), (Parshina et al., 2019) and (Kim & Gilmore, 1999).

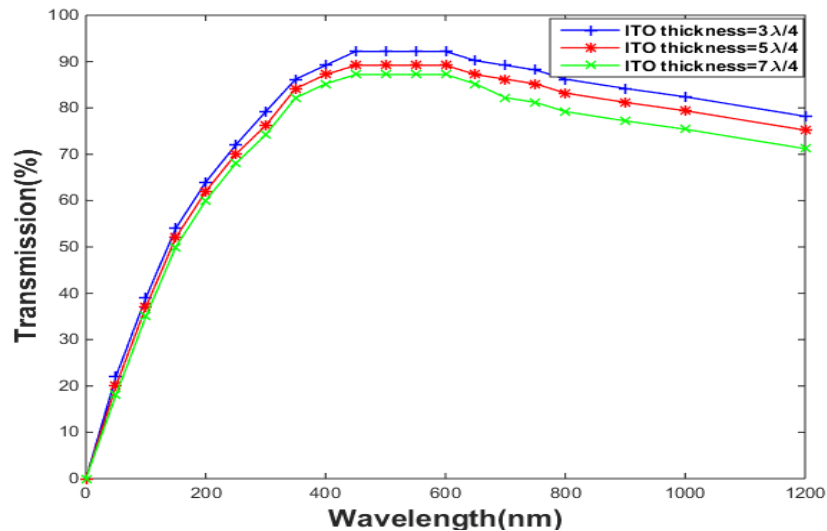


Figure 3: Simulated works of ITO films transmission with respect to thickness

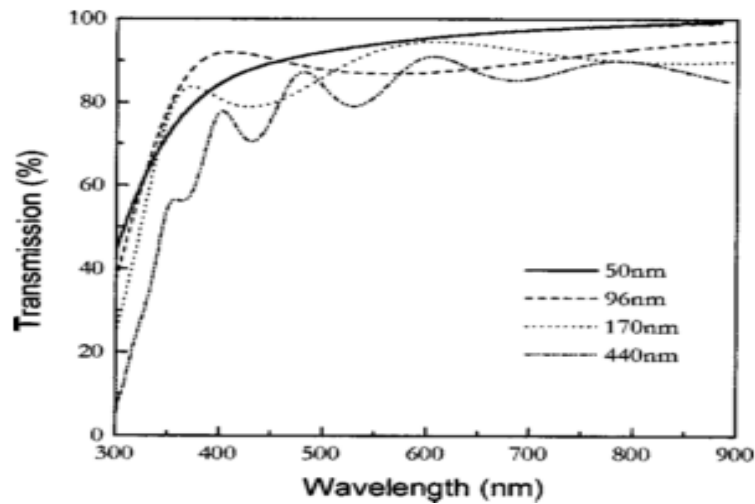


Figure 4: Experimental works of Guillén & Herrero (2007) ITO films transmission with respect to thickness

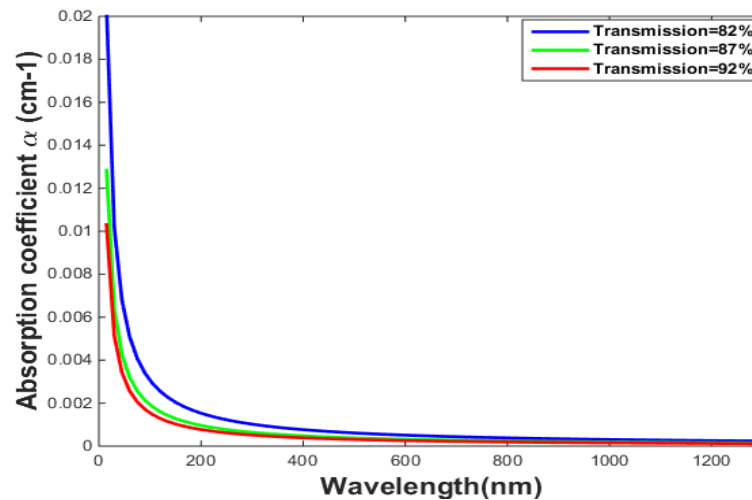


Figure 5: Optical absorption

Wavelength dependent ITO films optical absorption coefficient was computer-generated using absorption model (Eqn. 7), ITO refractive index n , m value, wavelength range of 0 to 1300 nm, and transmission from 81 to 92 % respectively. The experimental absorption graph of Thirumoorthi et al. (2016) was fitted with absorption model for absorption parameters evaluation. Fig 5 shows the simulated absorption coefficient with respect to decreasing optical transmittance. The result reveals a decrease in absorption coefficient as the ITO films transmission of energy is increased. Light energy absorption becomes very low when a large part of the energy is transmitted. Absorption of all the films from the graphs is in the range of 0.04-1.10% in the visible region. Furthermore, it can be seen that absorption edges shifted toward lower (energy) wavelengths as the transmission increases which imply a possible enlargement in ITO films band gap energy with increasing transmittance (Ghorannevis et al., 2015) (L. J. Meng & Dos Santos, 1998).

4. Conclusions

A model equation for the reflectance, optical absorption and transmission we investigated using simulation method. High transmission of about 91 % in the visible region was obtained for film with lowest thickness whereas the film with largest film exhibits about 85 % in the same region revealing a low optical transmission. For a good ITO films, also optical reflectance decreases with the increasing film thicknesses. Similarly, large ITO films thickness brought about high scattering effects whereas the low thickness reduces the optical scattering effect.

The features of optoelectronics properties were simulated; reflectance transmittance of ITO shows ITO layers were thicker films do produce better reflectance compared to the thin layers of ITO. A thin layer of ITO thickness obtained a very high transmission, while low optical transmission, larger film thickness is observed. Conclusively, it is clear that optoelectronics properties of ITO depend on thickness of the thin films. Result obtained was in agreement with the experimental and theoretical work available by other researchers.

Reference

- Afre, R. A., Sharma, N., Sharon, M., & Sharon, M. (2018). Transparent conducting oxide films for various applications: A review. *Reviews on Advanced Materials Science*, 53(1), 79–89.
- Akinkuade, S., Mwankemwa, B., Nel, J., & Meyer, W. (2018). Structural, optical and electrical characteristics of nickel oxide thin films synthesised through chemical processing method. *Physica B: Physics of Condensed Matter*, 535(June 2017), 24–28. <https://doi.org/10.1016/j.physb.2017.06.021>
- Alsultany, F. H., Ahmed, N. M., & Matjafri, M. Z. (2014). Effect of varying film thickness on the properties of indium tin oxide films after temperature annealing. *International Journal of Enhanced Research in Science Technology & Engineering*, 3(6), 443–446.
- Benamar, E., Rami, M., Messaoudi, C., Sayah, D., & Ennaoui, A. (1999). Structural, optical and electrical properties of indium tin oxide thin films prepared by spray pyrolysis. *Solar Energy Materials and Solar Cells*, 56(2), 125–139. [https://doi.org/http://dx.doi.org/10.1016/S0927-0248\(98\)00151-2](https://doi.org/http://dx.doi.org/10.1016/S0927-0248(98)00151-2)
- Chen, Z., Li, W., Li, R., Zhang, Y., Xu, G., & Cheng, H. (2013). Fabrication of highly transparent and conductive indium-tin oxide thin films with a high figure of merit via solution processing. *Langmuir*, 29(45), 13836–13842. <https://doi.org/10.1021/la4033282>
- Cui, H. N., Teixeira, V., & Monteiro, A. (2002). Microstructure study of indium tin oxide thin films by optical methods. *Vacuum*, 67(3–4), 589–594. [https://doi.org/10.1016/S0042-207X\(02\)00236-1](https://doi.org/10.1016/S0042-207X(02)00236-1)
- Ghorannevis, Z., Akbarnejad, E., & Ghoranneviss, M. (2015). Structural and morphological properties of ITO thin films grown by magnetron sputtering. *Journal of Theoretical and Applied Physics*, 9(4), 285–290. <https://doi.org/10.1007/s40094-015-0187-3>
- Guillén, C., & Herrero, J. (2007). Structure, optical, and electrical properties of indium tin oxide thin films prepared by sputtering at room temperature and annealed in air or nitrogen. *Journal of Applied Physics*, 101(7). <https://doi.org/10.1063/1.2715539>
- Isiyaku, A. K., Ali, A. H., Ahmad, R. A., & Zulaika, B. (2017). *Optoelectronic simulation properties of transparent conducting indium tin oxide for solar cell application*. 9(3), 49–54.
- Isiyaku, A. K., Ali, A. H., & Nayan, N. (2019). *Effects of Laser Radiation on the Optical and Electrical Properties of ITO Thin Films Deposited by RF Sputtering*. 6, 1–6. <https://doi.org/10.13189/ujee.2019.061601>
- Kamarudin, H., Retnasamy, V., Keng, C. J., & Palianysamy, M. (2014). Reflectance analysis of sputtered indium tin oxide(ITO) using UV Lambda. *Applied Mechanics and Materials*, 680, 102–105. <https://doi.org/10.4028/www.scientific.net/AMM.680.102>
- Kaushik, D. K., Kumar, K. U., & Subrahmanyam, A. (2017). Metal-insulator transition in tin doped indium oxide



- (ITO) thin films: Quantum correction to the electrical conductivity. *AIP Advances*, 7(1), 1–12. <https://doi.org/10.1063/1.4974157>
- Kerkache, L., & Layadi, A. (2005). *Physical properties of RF sputtered ITO thin films and annealing effect* My IOPscience *Physical properties of RF sputtered ITO thin films and annealing effect* This content has been downloaded from IOPscience . Please scroll down to see the full text . View. (December). <https://doi.org/10.1088/0022-3727/39/1/027>
- Kim, H., & Gilmore, C. M. (1999). *Electrical , optical , and structural properties of indium – tin – oxide thin films for organic light-emitting devices*. 86(11), 6451–6461.
- Kim, H., Piqué, A., Horwitz, J. S., Mattoussi, H., Murata, H., Kafafi, Z. H., & Chrisey, D. B. (1999). Indium tin oxide thin films for organic light-emitting devices. *Applied Physics Letters*, 74(23), 3444–3446. <https://doi.org/10.1063/1.124122>
- Lam, W. Y. (2014). *HKBU Institutional Repository*.
- Meng, L., Gao, J., Santos, M. P., Wang, X., & Wang, T. (2008). *The effect of the ion beam energy on the properties of indium tin oxide thin films prepared by ion beam assisted deposition*. 516, 1365–1369. <https://doi.org/10.1016/j.tsf.2007.04.159>
- Meng, L. J., & Dos Santos, M. P. (1998). Properties of indium tin oxide films prepared by rf reactive magnetron sputtering at different substrate temperature. *Thin Solid Films*, 322(1–2), 56–62. [https://doi.org/10.1016/S0040-6090\(97\)00939-5](https://doi.org/10.1016/S0040-6090(97)00939-5)
- Mohamed, S. H., El-hossary, F. M., Gamal, G. A., & Kahlid, M. M. (2009). *Properties of Indium Tin Oxide Thin Films Deposited on Polymer Substrates*. 115(3), 704–708.
- Parshina, L. S., Novodvorsky, O. A., Khramova, O. D., Lotin, A. A., Khomenko, M. D., & Shchur, P. A. (2019). Laser Annealing of Thin ITO Films on Flexible Organic Substrates. *Semiconductors*, 53(2), 160–164. <https://doi.org/10.1134/S1063782619020192>
- Salehi, A. (1998). *The effects of deposition rate and substrate temperature of ITO thin films on electrical and optical properties*. 214–218.
- Schultz, L., Harris, V. G., Huot, J., & Fan, H. (2017). *OF OF ALLOYS ALLOYS AND AND COMPOUNDS*. 48. [https://doi.org/10.1016/S0925-8388\(17\)32644-0](https://doi.org/10.1016/S0925-8388(17)32644-0)
- Shirakata, S., Sakemi, T., Awai, K., & Yamamoto, T. (2003). *Optical and electrical properties of ZnO films prepared by URT-IP method*. 445(3), 278–283. [https://doi.org/10.1016/S0040-6090\(03\)01161-1](https://doi.org/10.1016/S0040-6090(03)01161-1)
- State, S., & Road, L. (1981). *Indium-tin-oxide transparent conducting coatings on silicon solar cells and their*. 4, 151–158.
- Taha, H., Jiang, Z., Henry, D. J., Amri, A., & Yin, C. (2018). *Improved mechanical properties of sol-gel derived ITO thin films via Ag doping*. 14(December 2017), 210–224. <https://doi.org/10.1016/j.mtcomm.2017.12.009>
- Thirumoorthi, M., & Thomas Joseph Prakash, J. (2016). Structure, optical and electrical properties of indium tin oxide ultra thin films prepared by jet nebulizer spray pyrolysis technique. *Journal of Asian Ceramic Societies*, 4(1), 124–132. <https://doi.org/10.1016/j.jascer.2016.01.001>