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Simulation Analysis of Ito Films Optoelectronic Properties

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--ABSTRACT--

The unique optical and electrical properties of indium tin oxide (ITO) films have been regarded as one of the prominent transparent and conducting oxides (TCO) films used as contact layer in several optoelectronic applications. ITO films optoelectronics properties were studied using a computer simulation method with respect to thickness. Developed mathematical models of ITO films optical and electrical properties were used to determine the trend features of the films with respect to thickness and wavelength. Improvement in optical transmission was observed as the films thickness decreases with film of low thickness exhibiting a maximum transmission of 91 % in the visible region. Electrical property improved with increasing thickness. Low electrical resistivity of 7.4 Ω-cm was obtained by film with small sheet resistance (10 Ω/sq). The remarkable features of the results suggest that the developed models are significant for understanding the trend features of ITO films optoelectronic properties.

Key words: *ITO; Matlab; simulation; Thickness; transmission; reflectance*

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I. INTRODUCTION

Indium Tin Oxide (ITO) films have been considered as one of the leading transparent and conducting oxides (TCO) films used as contact layer in optoelectronics applications due to their high optical transmittance and good electrical properties. It is a wide band gap (3.5-5.0 eV) material with an optical transmittance greater than 80 % in the visible region of the spectrum [1,2]. ITO is an n-type degenerate semiconductor, with low electrical resistivity (~1×10^{-4} Ω cm). The low electrical property of ITO films is attributed to large number of intrinsic oxygen vacancies and extrinsic Sn^{4+} doping in the material [2-5]. Among the optoelectronics devices that incorporate ITO films as contact layer are solar cells, light emitting diodes (LEDs), sensors, touch screen, liquid crystal displays and smart window [6-9].

Deposition technique plays an important role in obtaining ITO films of an improved optical and electrical properties. Several techniques have been used such as spray pyrolysis [8], electron beam evaporation [9], pulsed laser deposition [10], Sol-gel method [11], Chemical vapor deposition method [12] and radio frequency (RF)/direct current (DC) magnetron sputtering technique [1-2]. Typically, the as-deposited ITO films are largely amorphous in nature. The amorphousness of the films can be transformed into polycrystalline films with good electrical and optical properties when exposed to post temperature annealing treatments [2]. ITO films need to be highly transmittance and of better electrical properties in order to enhance the optoelectronic device performance. Choosing a finest ITO film thickness is vital for having a good films contact. It is found that, using an ITO film thickness above 300 nm led to a lower transmission though increased conductivity [2, 14-16]. Consequently, ITO films resistivity value increased as the film thickness is decreased to below 100 nm, hence there is necessity for thorough investigation. In this work, ITO films optoelectronic features with respect to thickness were studied using a Matlab program (simulation). A mathematical models were fitted with already published experimental works to extract data for efficient simulation results.

II. MODELS AND METHODS

Computer simulation method is used to explain the optoelectronic properties of ITO films using optical transmittance, reflectance and absorption, resistivity and thickness dependence developed models equations. The properties are highlighted theoretically using Matlab software program. For ITO films, optical transmittance T depends on the films optical thickness t_{opt} as shown in Eqn.3. The optical thickness given as [17],

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

where m is either 0 or an even integer, λ is the wavelength and n is the refractive index, which is around 2 (for ITO). Moreover, transmission coefficient is given by,

$T = exp(-\alpha t),$ (2)

where α represents optical absorption and hence, Eqn. 2 can be rewriting as,

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

Optical absorption is obtained by substituting Eqn.1 in 2 and is written as,

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

Similarly, optical absorption as a function of photo energy is obtained using Eqn.5,

$\alpha^2 = \left(hv - E_g\right)$ (5)

where hv is photon energy, and E_g stands for band gap energy. Thus, reflectance dependence coefficient is given by

$R + T = 1$

(6)

Then using Eqn. 3, the optical reflectance coefficient can be evaluated as follows;

$R + exp(-\alpha(m+1)\frac{\lambda}{4n}), = 1$

$R = 1 + \exp(\alpha t)$ (7)

Furthermore, the two important parameters that simulate the optimization of electrical and optical transmission properties of ITO films are optical thickness t and sheet resistance $R_{s.}$ The films sheet resistance is given as,

$R_s = \frac{\rho}{t} =$

(8)

By substituting $t = \frac{(m+1)\lambda}{4}$, then the films average electrical resistivity can be obtained as,

$\rho = \frac{R_S(m+1)\lambda}{4}$

(9)

Eqns. 1-9 were used to simulate the optoelectronics features of ITO films using MATLAB program. Optical absorption coefficient of range between 0 to 0.020, and wavelength range of 0 to 1000 nm were selected after a careful consideration of some research works [15-18].

III. RESULTS AND DISCUSSION

Fig. 1 shows the simulated ITO films optical transmission as a function of films thickness (3λ/4, 5λ/4 and 7λ/4) respectively. It is observed that the optical transmission increased with decreasing films thickness. Lowest transmission of 85 % at 550 nm wavelength was obtained by film with the highest thickness (7λ/4) whereas highest transmission of 91 % at 550 nm wavelength in the visible region was obtained by film with very thin ITO film thickness (3λ/4) and is found to be in conformity with an experimental result of [19-21,26]. The improved optical transmission is attributed to possible particles growth, loss of light arising from oxygen vacancies and reduction in films defects with decreasing films thickness [1, 2, 5].

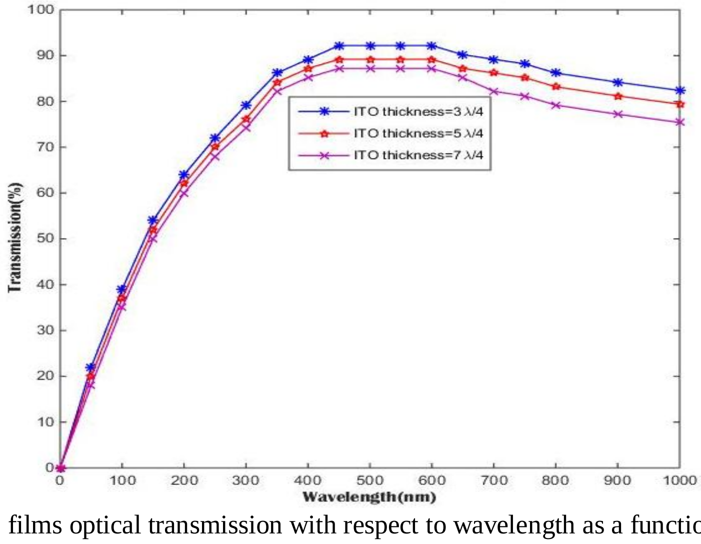

Fig. 1: ITO films optical transmission with respect to wavelength as a function thickness

Fig.2 displays the ITO films optical reflectance as a function of 3λ/4, 5λ/4 and 7λ/4 thickness respectively. The figure shows a decreased in reflectance as the films thickness is decreased. For optimum performance of optoelectronics devices, ITO films contact must have low optical reflectance for maximum transmission of light. the large ITO films thickness brought about high scattering effects whereas the low thickness reduces the optical scattering effect for enhance transmission and this reflectance thickness phenomena was similarly highlighted in the experimental works of Kamarudin et al. (2014) and Salehi (1998) respectively [20,21].

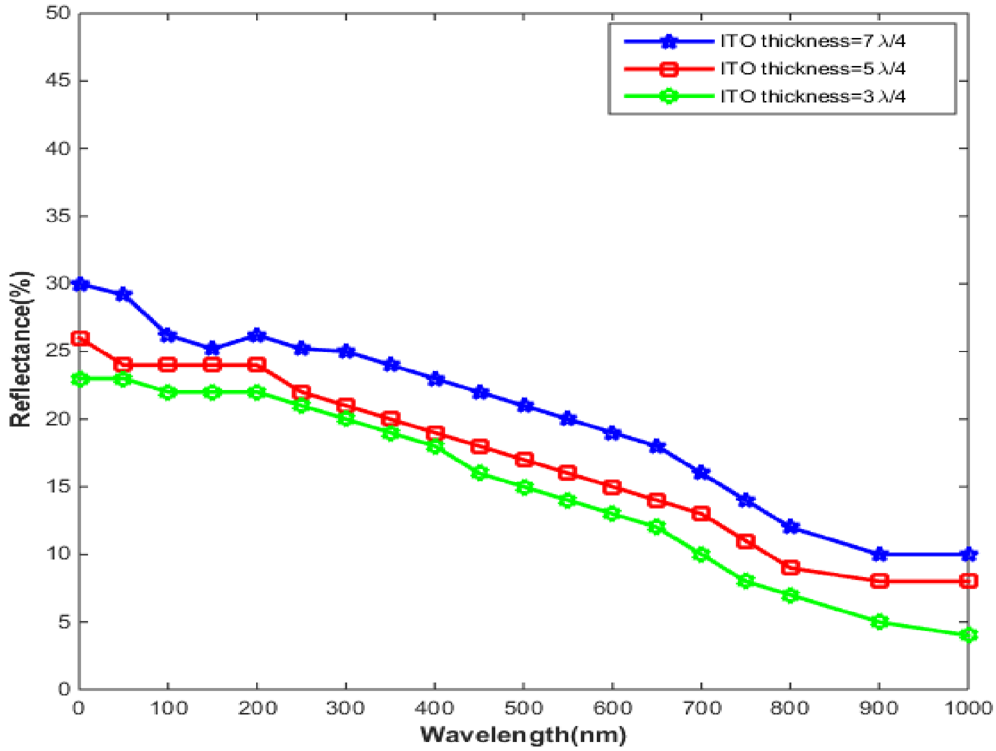

Fig. 2: ITO films optical reflectance with respect to films thickness

ITO films band structure is vital since it estimates the amount of photon energy absorbed. Fig. 3 shows the ITO films absorption coefficient against photon energy as a function of band gap energies 3.69 eV, 3.80 eV and 3.92 eV respectively. For ITO films we assumed a direct transition in order to find the band gap energy (using Eqn. 5) [23]. The ITO films band gap energies were obtained after extrapolating the linear plots at zero absorption coefficient. It can be observed that the films band gap energy increases with an increasing photon energy. The maximum gap energy of 3.92 eV is attributed to ITO films with high photon energy whereas the minimum energy gap of 3.62 eV is associated with films with low photon energy absorption. Moreover, it is noted that high photon energy is achieved when there is high optical transmission

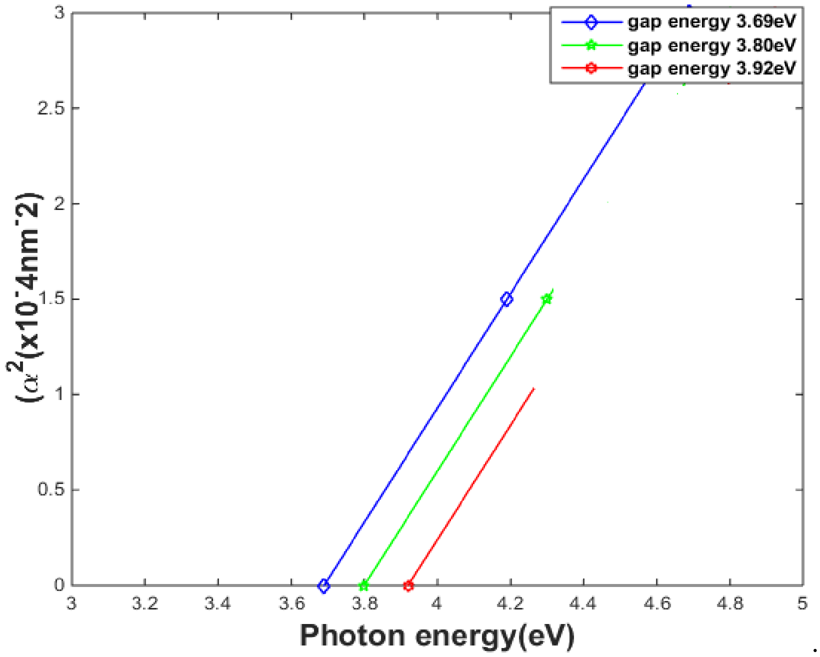

Fig. 3: Simulated absorption coefficient variation with photon energy.

The ITO films electrical conductivity characteristics with respect to resistivity and sheet resistance were estimated using a theoretical approach and compared with the published experimental findings. Fig.4 shows the simulated ITO films electrical resistivity as a function of sheet resistance (10 Ω/sq, 14 Ω/sq, 16 Ω/sq). In this work, the experimental resistivity graph of Patel et al., 2003 was fitted with the resistivity model in Eqn.9. A substantial enhancement in electrical resistivity was observed with decreasing sheet resistance. The ITO films resistivity value decreased as the sheet resistance value is increased. This is in agreement with the experimental result of Patel at al., 2003. Low sheet resistance of 10 Ω/sq corresponded to 7.4 Ω-cm resistivity at 550 nm wavelength in the visible region. The enhancement in resistivity can be attributed to the increase in grain size with increasing thickness or post annealing temperature which at same time resulted in decrease of grain boundary scattering effect [2, 26, 27]. The low sheet resistance and resistivity at this wavelength is required to get a high electrical conductivity for improve optoelectronic devices such as solar cells.

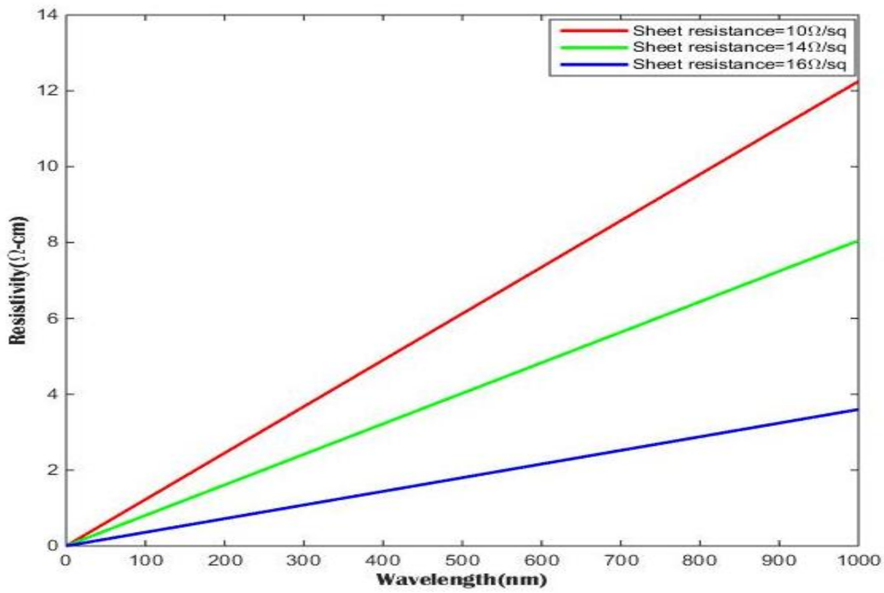

Fig. 4: ITO films simulated resistivity as a function of increasing sheet resistance

Fig. 5 shows the ITO films simulated resistivity variation with thickness (using Eqn.9). It can be noted that the resistivity value reduces with the increasing films thickness. Also an increase in resistivity is observed with decreasing m value, which determine the film thickness. This showed that thinner (low) films have a high resistivity value compared to thicker films which is in consistent with the some experimental research works [26,27].

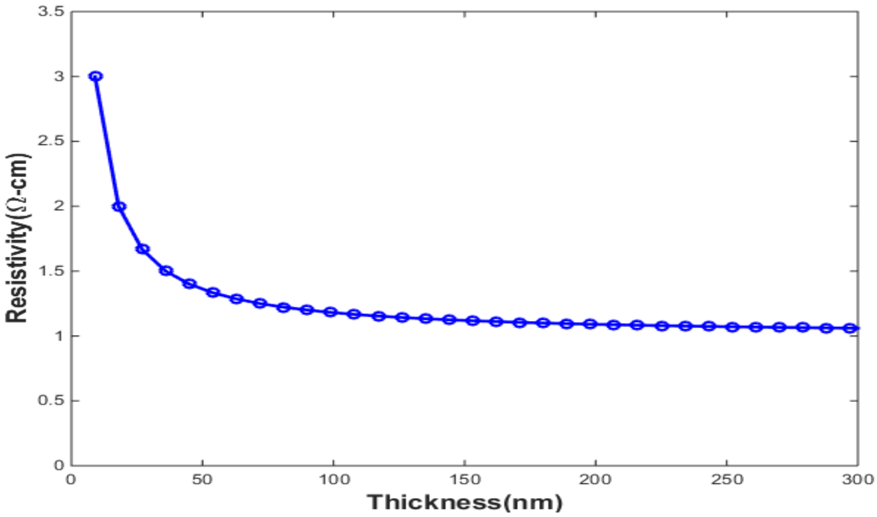

Fig. 5: ITO films resistivity against optical thickness

IV. CONCLUSION

ITO films optoelectronics features were investigated using theoretical approach (Matlab program). Developed simulation models were used to highlight the films optical transmission, reflectance, absorption and electrical properties with respect to thickness. The results show that the films optical property enhances as the thickness increased whereas electrical property improved with increasing thickness. Maximum transmission of 91 % at 550 nm wavelength was obtained by film with lowest thickness (3λ/4). Minimum sheet resistance of 10 Ω/sq produces the lowest resistivity value of 7.4 Ω-cm. these simulated ITO films optical and electrical properties are promising films (contact) for any low resistance optoelectronic devices such as solar cells.

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