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Optoelectronic simulation properties of transparent conducting indium tin oxide for solar cell application

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Abstract: The flexible and unique features of indium tin oxide (ITO) have continued to qualify this material for used in wide range of optoelectronic applications. Optical and electrical properties of indium tin oxide were investigated using a computer simulation (Matlab program). Derived models of ITO comprising transmission, resistivity and optical absorption were used to examine and validate the trend features of the ITO transparent conductive material. All the models parameters used in this study were within the limit range values of the material and have found to affect changes in the electronic and optical properties of indium tin oxide. Data obtained in this work were compared with the experimental findings. The attractive features of the results indicate that the models used can be further manipulated to extract other parameters such as reflectance and temperature dependent transmittance.

Keyword: Indium tin oxide; Simulation; Matlab; Resistivity; Optical absorption; transmission.

1. Introduction

Indium tin oxide (ITO), a transparent conducting oxide has been studied extensively for many decades because of its excellent transparency and conducting properties [1]. ITO In_2O_3: Sn is a wide band gap (3.3-4.3 eV) and highly degenerate *n-type* semiconductor material [1-2]. The high transparency of ITO thin films in the visible and near infrared regions of the spectrum is attributed to the increasing band gap energy [3]. In_2O_3:Sn conductivity or degeneracy is due to the oxygen vacancy and doped tin extrinsic defect [4]. Many optoelectronics device applications use indium tin oxide as transparent conducting electrodes such as organic light emitting diode [5], solar cell [6], and plasma display panel [7]. ITO is used as front contact and anti-reflection coating in solar cells devices [8]. The use of a small absorbing front and rear back ITO contacts led to the improved conversion efficiency of thin film solar cells [5,15].

Different fabrication techniques have been used to deposit ITO on a substrate, including direct current (dc) and radio frequency (rf) magnetron sputtering [7],chemical vapor deposition [9], sol gel method [10] ion beam assisted deposition [2], pulsed laser deposition [1], plasma ion assisted evaporation [11], electron beam deposition [6], spray pyrolysis [12] and thermal evaporation [13]. Sputtering technique is mostly used to deposit ITO thin film due to unique results that have been obtained using this method. High quality and exceptional thin films deposited over a large area have also been obtained by sputtering method [7,14].

Band gap energy and absorption coefficient are the two relevant parameters that play significant roles in the optimization of ITO transmission in the visible range and lowering of electrical resistivity. Tuna *et. al.* report a correlation between band gap, absorption coefficient, substrate temperature, transmission, and resistivity [7]. As the gap energy increases, resistivity decreases with respect to an increase in substrate temperature. Increase in substrate temperature widens the band gap and subsequently increases the carrier concentrations. Higher transmission is also obtained when band gap of thin ITO Films widened. The absorption coefficient is found to be decreasing with increasing incident photon energy. In this work,

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optoelectronic features of ITO films for solar cells application are studied using a theoretical approach.

2. Models and Methods

The simulation method is adopted in this work to explain the flexible features of ITO films using optical transmission, resistivity and absorption developed models equations. The requirements for applications of transparent conducting ITO films in photovoltaic devices are estimated and highlighted theoretically using Matlab software program. Higher transmissivity and conductivity couple with a very low electrical resistivity are required for a good ITO films for application in solar cells [16]. Hence, optical transmission T of transparent conducting oxide depends on the films optical thickness t_{opt} and is given by Eq. (1),

$$T = \exp\left(-\alpha t_{opt}\right) \tag{1}$$

where α is the optical absorption [1,8]. Indium tin oxide is used as front contact in solar cells, due to its high transmittance and conductivity in the visible and near infrared region [17]. It also serves as antireflection coating [8,15]. Optical thickness of transparent thin films for achieving antireflection properties is a wavelength dependent as given in Eq. (2),

$$t_{opt} = (m+1)\frac{\lambda}{4n} \tag{2}$$

where m stands for either 0 or even integer, λ is the wavelength and n represent refractive index [8]. Eq. (1) is re-modeled by substituting Eq. (2) in (1).

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

Sheet resistance R_s and thickness t are the two important parameters that stimulate the optimization of optical transmission and electrical conductivity of any transparent conducting films [18-19]. Sheet resistance of any transparent conducting film is found to be inversely proportional to the thickness of the same films [8, 20],

$$R_s = 1/\sigma t \tag{4}$$

where σ is the average electrical conductivity of the film. The resistivity ρ and thickness t, $t = (m+1)\frac{\lambda}{4}$ of the coating film are related as in Eq. (5) [8],

$$\rho = R_s \times (m+1)\frac{\lambda}{4} . \tag{5}$$

Optical transmission and wavelength dependent absorption coefficient is obtained by substituting t in Eq. (1).

$$\alpha = \frac{4}{(m+1)\lambda} lin\left(\frac{1}{T}\right) \tag{6}$$

The photon energy related optical absorption coefficient used for estimation of optical band gap energy is given by Eq. (7) [21].

$$\alpha^2 = (hv - E_g) \tag{7}$$

Optical absorption coefficient and the wavelength range of 0-0.020 cm^{-1} and 0-800 nm are selected after careful evaluation of ITO films features from the work of other researcher [27, 31-32]. The absorption properties were simulated using Eq. (6) and (7). Even integers m values that determine the thickness and resistance range (6-8 Ω/sq.) required for ITO thin films application in photovoltaic devices are used. The transmission trends with respect to thickness and wavelength dependent resistivity were also run in Matlab program.

3. Results and Discussion

Majority of the works on ITO films centered at the improvement of the optical and electrical properties concurrently [20,22]. Wavelength dependent optical absorption coefficient is simulated using Eq. (6) in Fig. 1. The result reveals a decrease in absorption coefficient as the transmission of energy through ITO films increases. Light energy absorption becomes very low when a large part of the energy is transmitted. This indicates that indium tin oxide is a wide band gap material in which high transparency is produced as a result of direct and wide band gap state of the material [19, 23]. ITO maximum transmittance and low energy absorption are the two important properties for application in solar cells [24].

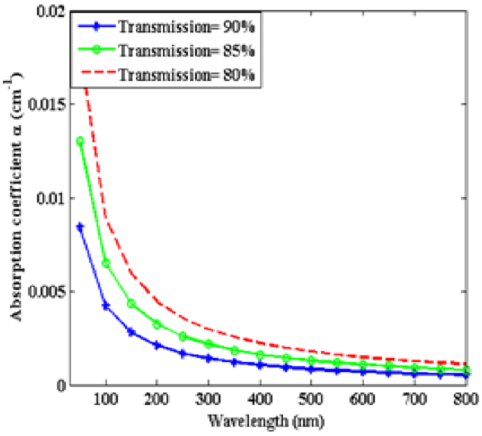

Fig. 1 Wavelength dependent optical absorption coefficient.

Good transparent conducting oxides possess high transmission abilities as well as low resistivity for use in solar cells. Fig. 2 presents the trend of transmission of ITO thickness with respect to wavelength. High transmission is obtained for very thin ITO thickness while larger films thickness reveals low optical transmission as also indicated in the work of Cui *et. al.* [30]. Maximum transparency is reached at wavelength range 450-600 nm. This range of high transmission wavelength is required for ITO films to serve as a good antireflection coating [8].

Knowledge of energy band structure that determines the amount of photon energy absorbed is crucial to understand the optical properties of the materials [25, 26]. Fig. 3 and 4, show the calculated extrapolated linear plots of optical band gaps of ITO films from the simulation and work of Meng and Santos, (1998) for comparison. The energy gap of 3.92 eV is attributed to ITO with smaller thin film nano meter grain size and higher surface roughness, while the 3.5 eV is associated with ITO of increasing film grain size caused by the quantum confinement effect [28]. Higher energy band gap corresponds to lower photon energy absorption for the ITO thin films.

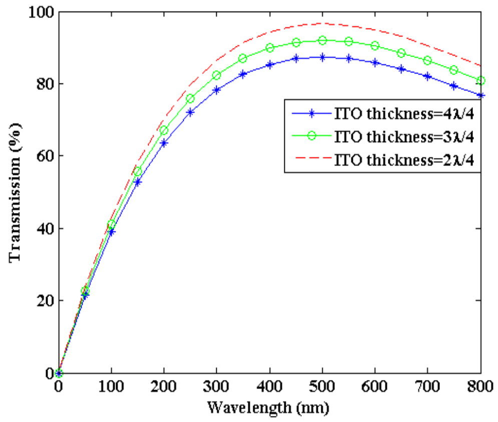

Fig. 2 Wavelength dependent transmission.

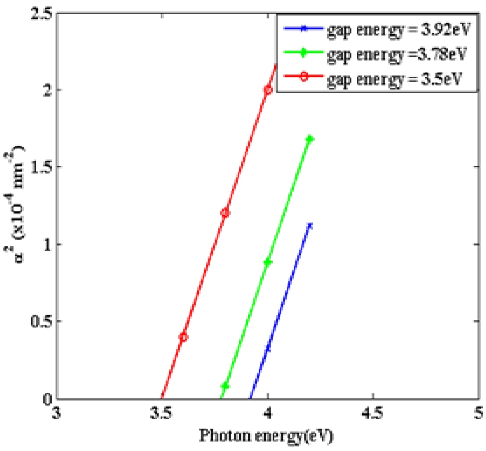

Fig. 3 Simulated absorption coefficient variation with photon energy.

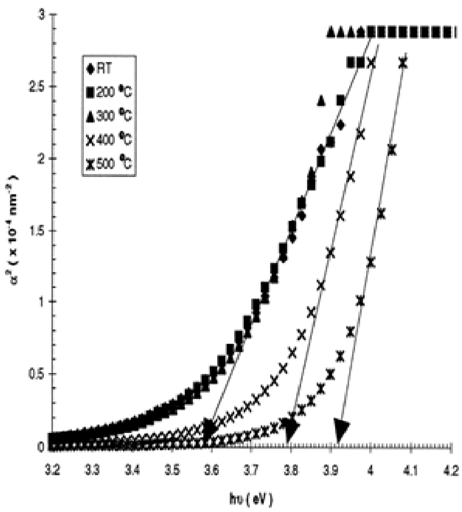

Fig. 4 Calculated absorption coefficient variation with photon energy.

Electrical performance of ITO films is evaluated by the state of sheet resistance of the films [20]. Sheet resistance for displays and thin film solar cells devices should be as low as possible [19, 29]. Fig. 5 highlighted the calculated resistivity ρ of the films (Eq.5), knowing the sheet resistance *Rs* (6 Ω/s, 8 Ω/sq, and 12 Ω/sq) and the wavelength range that extends to infrared region. A calculated ITO samples of 32.5 Ω/sq and 448.8 Ω/sq for ITO/Ni/ITO and single ITO films respectively is presented in Fig. 6 for comparison [19]. In both the results, the uniform increment of resistivity with respect to wavelength and film thickness is obtained. Low sheet resistance reveals a very low but uniform resistivity. The trend features of this calculated experimental work of Yun *et al*. validated our finding [19].

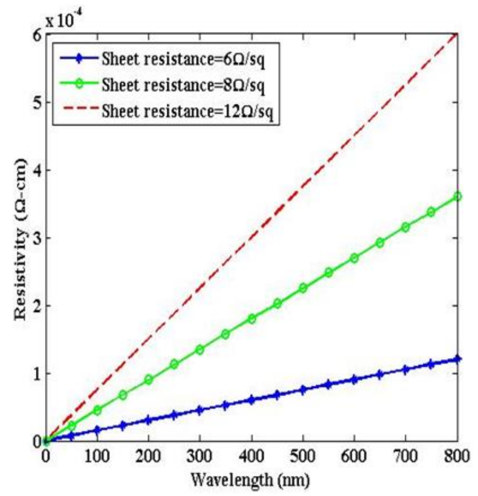

Fig. 5 Variation of resistivity with respect wavelength for decreasing sheet resistance.

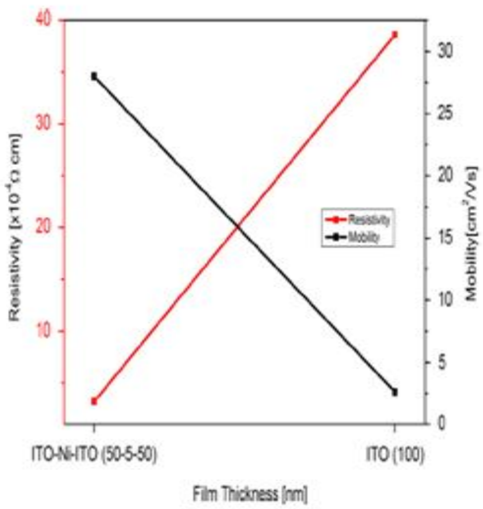

Fig. 6 Variation of Resistivity with film thickness.

4. Conclusion

The transparency and conductivity features of indium tin oxide films were investigated using a simulation method. The substitutional models of transmission, optical absorption coefficient and resistivity were used to highlight the fundamental features of ITO thin films. Transmissions of light energy through the ITO films are found to be thickness, band gap energy, and absorption coefficient dependent. Higher band gap and low optical absorption result in the maximum transmission of light energy while increasing films thickness exhibited low transmissivity. The electrical conductivity performances were shown to be a function of sheet resistance. The resistivity of ITO films progresses uniformly with respect to wavelength or thickness for decreasing sheet resistance. Low sheet resistance corresponds to small resistivity which is a good estimate for application in solar cells. In general, these developed models were able to explain the experimental observation of ITO films, thereby validating the simulated findings.

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