IEEE Access
Multidisciplinary : Rapid Review : Open Access Journal

Received 12 February 2023, accepted 1 March 2023, date of publication 6 March 2023, date of current version 13 March 2023.

Digital Object Identifier 10.1109/ACCESS.2023.3252890

RESEARCH ARTICLE

Experimental Investigation and DFT Study of Tin-Oxide for Its Application as Light Absorber Layer in Optoelectronic Devices

MANOJ KUMAR[1], SYED SADIQUE ANWER ASKARI[2], PURNENDU SHEKHAR PANDEY[3], (Senior Member, IEEE), YADVENDRA SINGH[4], (Member, IEEE), RAJESH SINGH[5,6], (Member, IEEE), SANJEEV KUMAR RAGHUWANSHI[2], (Senior Member, IEEE), GYANENDRA KUMAR SINGH[7], AND SANTOSH KUMAR[8], (Senior Member, IEEE)

[1]MLR Institute of Technology, Hyderabad 500043, India
[2]Department of Electronics Engineering, Indian Institute of Technology (Indian School of Mines) Dhanbad, Dhanbad, Jharkhand 826004, India
[3]Department of Electronics and Communication Engineering, GL Bajaj Institute of Technology and Management, Greater Noida 201306, India
[4]School of Electrical Engineering and Computer Science, Oregon State University, Corvallis, OR 97331, USA
[5]Uttaranchal Institute of Technology, Uttaranchal University, Dehradun 248007, India
[6]Department of Project Management, Universidad Internacional Iberoamericana, Campeche 24560, Mexico
[7]Department of Mechanical Engineering, School of Mechanical, Chemical and Materials Engineering, Adama Science and Technology University, Adama 1888, Ethiopia
[8]Shandong Key Laboratory of Optical Communication Science and Technology, School of Physics Science and Information Technology, Liaocheng University, Liaocheng 252059, China

Corresponding author: Gyanendra Kumar Singh (gyanendra.kumar@astu.edu.et)

This work was supported by the Science and Engineering Research Board, Department of Science and Technology, Government of India, for the project titled "Design of a web server-based hybrid physiological sensor with optical cloth for real-time health specialist care" (August 2022) under Project SCP/2022/000271.

ABSTRACT Experimental investigation of Tin Oxide (SnO) film has been performed to analyse the effect of oxygen ratio variation on its optical and electrical properties. The oxygen composition in SnO film has been varied and correspondingly its extinction coefficient and band gap have been obtained. Also, density functional theory (DFT) study of SnO film has been carried out in order to obtain its optical properties such as extinction coefficient and corresponding bandgap. The experimental and theoretical trends related to its optical properties are in good agreement with each other. The SnO film may be used as a prospective light absorber layer in various opto-electronic sensor devices, solar cell in particular, and its optoelectronic properties can be tuned with change in oxygen mole fraction ratio of SnO films which are detailed out in this paper. Further, some important electrical parameters of such as Hall mobility, carrier concentration and resistivity of SnO films for its different Sn and O ratios have been obtained. The investigation of tunable optical and electrical properties of SnO thin film will pave the way for a wide range of opto-electronic devices.

INDEX TERMS Oxide semiconductors, optical properties, SnO, DFT, e-beam.

I. INTRODUCTION

In order to be used in wide range of photonic devices, metal oxide semiconductors have been the subject of intensive research for many years. This is due to their extraordinary versatility in opto-electronic properties and their ability to grow at low temperatures [1]. Metal oxides (MO_x) are one type of material that has piqued the interest of optoelectronic researchers due to their scalable development techniques and customizable material properties such as band gap and conductivity [2], [3]. Metal oxides can operate as semiconductors exhibiting either n- or p-doped nature, depending on whether they are intrinsically or extrinsically doped. Metal oxides are also appealing because they are stable, non-toxic, and can be

The associate editor coordinating the review of this manuscript and approving it for publication was Sukhdev Roy.

manufactured using low-temperature techniques. Moreover, use of metal-oxides as carrier selective contacts namely TiO_2, ZnO, SnO_2 etc. as electron transport layer and V_2O_5, WO_3, MoO_3, NiO as hole transport layer for organic solar cells has also been reported. But, some metal-oxides have the potential to be used as light absorber layer which can be used for opto-electronic devices. Owing to the tunable band gap these oxides may be made suitable for absorbing visible spectrum of light. However, there are just a few oxide semiconductors with good hole transport characteristics, configurable band gaps, and light absorption in the solar spectrum [4], [5]. Copper oxide (CuO), Cobalt oxide (CoO) and Iron oxide (FeO) are among the few binary compound oxide semiconductors capable of absorption of visible solar spectrum light. Furthermore, its extensive application in the opto-electronic sectors is constrained by the need for high growth temperatures (600 ^{o}C for the growth of CuO film) and expensive procedures like ALD and MBE (for the growth of CoO and FeO film) [2]. Researchers must therefore focus on tin-oxide-based semiconductors since they demand low growth temperatures as well as an easy and affordable fabrication procedure. Over the decades, tin-dioxides (SnO_2) have been explored to reveal its potential to be used in a wide range of applications, including electro catalysis, transparent conductive electrodes, electrochromic devices, and solar energy conversion [6], [7], [8]. Furthermore, tin-oxides (SnO) have been studied recently by a few researchers for use in organic solar cells, thin film transistors, hole transport layers, etc., [9]. According to studies, important SnO features like band gap, carrier concentration, mobility, etc., vary drastically with the increasing oxygen compositional ratio in SnO film [10], [11], [12]. Wavelength dependent extinction coefficient and bandgap of SnO are some of important parameters owing to its application as light absorber layer for photosensitive devices. Generally, excessive increase in oxygen (O) or tin (Sn) vacancies lead to localized states lying around the Fermi level which are often terms as structural defects [13], due to which some important parameters such as carrier mobility get reduced [14], which may leads to increase in electrical resistivity of SnO samples. Also, some unwanted intra-band photon absorption in a SnO crystal increases due to which photo generation rate may be affected [15]. However, owing to oxygen vacancies in metal oxide semiconductors often results in change in its carrier concentration and nature (n-type or p-type). Therefore, vacancies, oxygen (O) vacancy in particular, in a metal oxide (here SnO) semiconductor should be optimized in order to get optimum value of carrier concentration, resistivity, mobility along with desired optical absorption. Moreover, dependency of tin and oxygen ratio on its extinction coefficient and band gap studies of the SnO film needs to be explored in order to find its usage in wide range of optoelectronic devices [8], [16], [17]. In this work, optical properties such as extinction coefficient and band gap studies of the SnO thin film have been theoretically and experimentally studied.

II. DESIGN CONSIDERATION

In this work, the CASTEP toolkit package were employed to perform the band structure and optical properties calculation of SnO super cell [18].The calculations were performed using generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) functional by norm-conserving pseudopotentials of Cambridge Sequential Total Energy Package code (CASTEP) tool kit of Material Studio. The convergence tolerance parameters value were set to be as 830 eV as cutoff energy for the k-point fine mesh of $5\times 5 \times 8$, maximum force, maximum stress and maximum displacement were set to be 0.03 eV/A^0, 0.05 GPa and 0.001 A^0, respectively. The SCF tolerance value was considered to be fine, i.e., 10^{-6} eV/atom. The optical properties (extinction coefficient), XRD and band gap of SnO films for its different tin and oxygen compositional ratio have been extracted using CASTEP toolkit of Material Studio by using aforementioned parameters. The structure of SnO (tetragonal; P4/nmm; 129) super cell as shown in Figure 1(a) has been imported from the inorganic crystal structure database of material studio. In Figure 1, Tin (Sn) atoms are represented by gray colored balls and oxygen (O) atoms are shown by red balls. Some additional interstitial oxygen atoms have been incorporated in the SnO super cell at its lattice sites of in order to relatively increased the oxygen content in SnO super cell as shown in Figure 1(b). Similarly, the oxygen content of SnO super cell at its lattice sites is further increased by incorporation some additional oxygen atoms as shown in Figure 1(c) which shows relatively highest amount of interstitial oxygen atoms in SnO super cell as compared to Figure 1(a) and (b). Thus, qualitatively assuming the SnO super cell as shown in Figure 1 (a) to have tin and oxygen (Sn:O) ratio as 1:1, Sn:O ratio of Figure 1 (b) as 1:2 and Sn:O ratio of Figure 1 (c) as 1:3.

III. GROWTH OF SnO THIN FILMS

The experimental works related to the growth of tin-oxide (SnO) have been carried out using customized e-beam (electron-beam) deposition system (shown in Figure2(a)) by regulating the growth oxygen pressure through mass flow controller (MFC) of e-beam chamber as shown in Figure2 (b). Tin (Sn) pellets (purity of 99.9 %) are placed in Molybdenum crucible which were evaporated by e-beam and reacts with oxygen atoms present inside the chamber to form SnO film in the vicinity of glass substrate at room temperature. Qualitatively, the compositional ratio of Sn and O have been altered during experimental growth of SnO film by varying growth oxygen pressure inside e-beam chamber, e.g., 1:1 ratio of Sn and O denotes the flow rate of O (oxygen) inside chamber to be 1 sccm (standard cubic centimetres per minute), 1:2 denotes the flow rate of O (oxygen) to be 2 sccm and similarly, 1:3 denotes the flow rate of O (oxygen) to be 3 sccm.

IV. RESULTS AND DISCUSSION

The structural property such as XRD patterns, optical properties (extinction coefficient, transmittance) and band gap of SnO films for its different tin and oxygen compositional

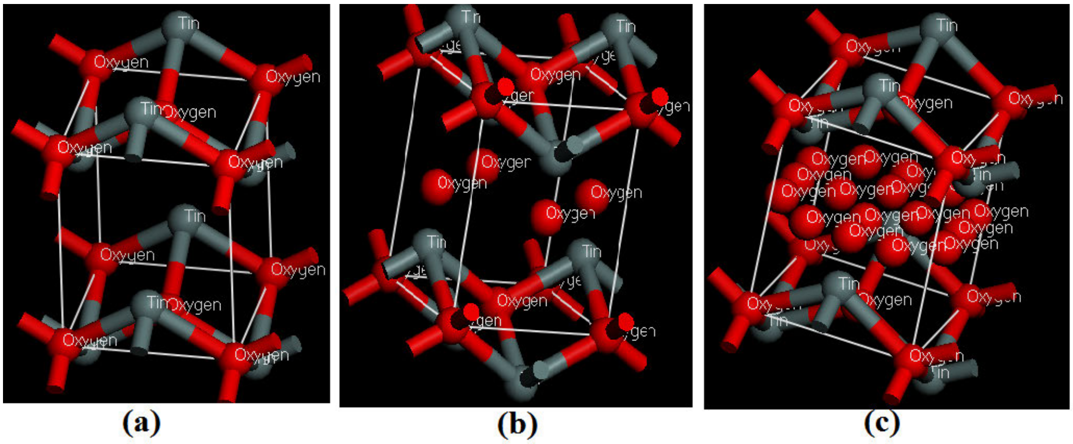


FIGURE 1. (a) SnO super cell (b) SnO super cell having interstitial oxygen atoms (c) SnO super cell having relatively higher interstitial oxygen atoms.

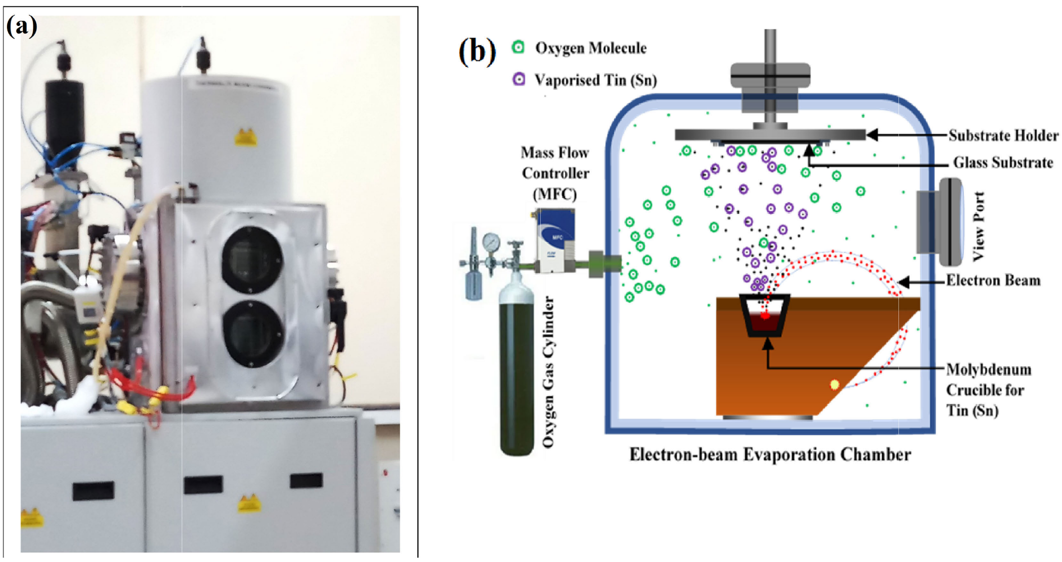


FIGURE 2. (a) Customized e-beam chamber (b) Schematic layout of e-beam process.

ratio have been extracted experimentally as well as it have been simulated using CASTEP toolkit of Material Studio according to aforementioned parameter details as mentioned in section II.

Figure 3(a-f) shows the room temperature XRD patterns of SnO films for its different Sn:O compositional ratios. Experimentally, XRD patterns were obtained by X-ray diffractometer (Rigaku, SmartLab). The experimentally obtained XRD patterns were compared with simulated results of XRD patterns (shown in Figure 3(d-f)) obtained from XRD toolkit of material studio. From experimental as well as simulated XRD pattern, it is found that maximum peak is obtained at $2\theta = 30.50$ and 48.140 which corresponds to SnO peak which confirms the existence SnO phase. As the oxygen ratio in SnO increases, then along with some SnO peaks, there are also existence of few SnO_2 peak at $2\theta = 65.50$ and 74.140 as shown in Figure 3(b-c). It is primarily because of increase in rate of oxidation of SnO film due to increment in oxygen flow inside e-beam chamber during growth of SnO film. The enhanced rate of oxidation converts Sn^{2+} to Sn^{4+} oxidation states which corresponds to formation of SnO_2 phase [27], thus some amount of SnO_2 are also formed along with SnO peak as shown in Figure 3(b-c) which corresponds to experimental XRD patterns of SnO films. For the sake of clarity to identify the important peaks, XRD patterns of SnO films as mentioned above, have been compared with standard (JCPDS-Joint Committee on Powder Diffraction Standards) SnO, and SnO_2 diffraction patterns [28], as shown in Figure 3(a-f). It may be mentioned here that as per the technical reports available in literatures, it is shown that SnO are thermally stable under normal atmospheric condition at room temperature [29]. The existence of Sn^{2+} ion of SnO at room temperature can also be confirmed by our XRD pattern of SnO thin film as shown in Figure 3(a-c), which has been carried at room temperature under normal atmospheric condition. Moreover, at elevated temperatures, i.e., beyond 300^{o}C, Sn^{2+} state of SnO has high probability of getting converted to Sn^{4+} oxidation

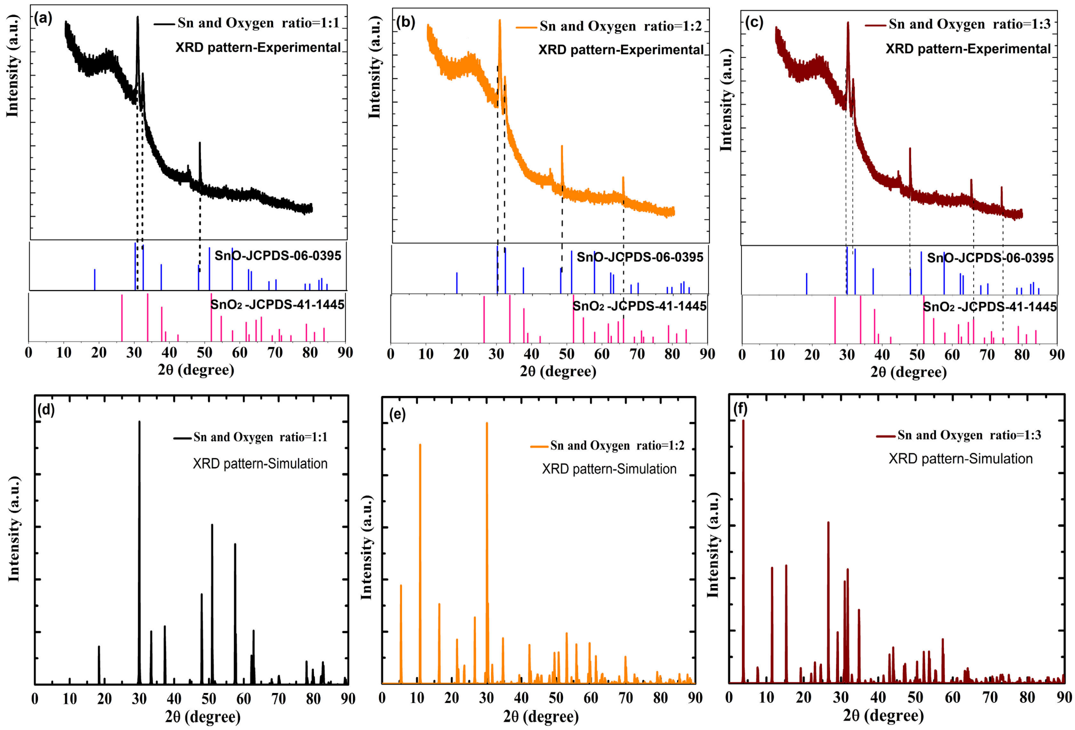


FIGURE 3. XRD patterns of SnO films for its different Sn;O compositional ratios: (a-c) Experimental and (d-f) Simulation.

state but at room temperature Sn^{2+} state of SnO remain stable [29].

The density functional theory (DFT) results of SnO film shows that with an increase in Sn:O ratio, i.e., relative increase in amount of oxygen atoms with respect to Sn atoms in crystal, the extinction coefficient of SnO decreases (shown in Figure 4), whereas the bandgap of SnO film (shown in Figure 5) increases with an increase in Sn:O compositional ratio. In order to verify the trend of extinction coefficient and band gap variation of SnO film with change tin and oxygen composition ratio, the results obtained from DFT study of SnO film have been compared with experimentally obtained extinction coefficients and band gaps of SnO film.

The optical characterization of SnO samples having different Sn:O compositional ratios have been carried out using UV-VIS-NIR spectrophotometer. Extinction coefficient (k) (shown in Figure 4(a) are calculated from measure values of reflectance spectra R(λ) and transmittance spectra T(λ) by UV-VIS spectrophotometer, using the following formulae Eq. 1 and Eq. 2 [26].

$$k = \left[\frac{\alpha(\lambda)\lambda}{4\pi}\right] \quad (1)$$

$$\alpha(\lambda) = \frac{1}{d} * [ln\left\{(1 - R(\lambda))^2/T(\lambda)\right\}] \quad (2)$$

where d is thickness of SnO film, R(λ) and T(λ) are wavelength dependent reflectance and transmittance spectra of SnO film, respectively.

Simulated as well as experimental value of extinction coefficient of SnO films for its different composition of Sn and O ratios have been shown in the Figure 4. From the Figure 4, it is observed that the extinction coefficient of SnO samples, firstly increases with increase in wavelength of light, particularly at shorter wavelength (500 nm <) and thereafter extinction coefficient decreases at higher wavelength. Theoretically, it can be stated that photons having higher wavelengths have lower energy than that of photons having shorter wavelengths. Therefore, absorption of shorter wavelengths photons for a given band gap of SnO are more as compared to longer wavelength consequently extinction coefficient increases for shorter wavelength and decreases with increase in wavelength of photons as shown in Figure 4(b). However, from the experimentally obtained extinction coefficient (shown in Figure 4(a)) graph, it can be observed that first, the value of extinction coefficient firstly increases and then decreases after a particular wavelength that is beyond 500 nm. Practically, thickness of thin film plays important role in constructive and destructive inference phenomenon of incident photons on the surface of thin film, due to which the thin film absorption and hence extinction coefficient shows maximum value at particular wavelength due to constructive interference [30]. Both experimental and simulated results of extinction coefficient of SnO sample shows that extinction coefficient decreases with increase in its compositional (Sn:O) ratio. This is mainly due to the fact that with an increase in Sn:O ratio, oxidation process inside the growth chamber is proportionally increased, and thus transparency of SnO film increases as shown in Fig. 6(a) and hence, extinction coefficient of SnO film decreases. But at shorter wavelength, i.e., wavelength less than 500 nm, trend

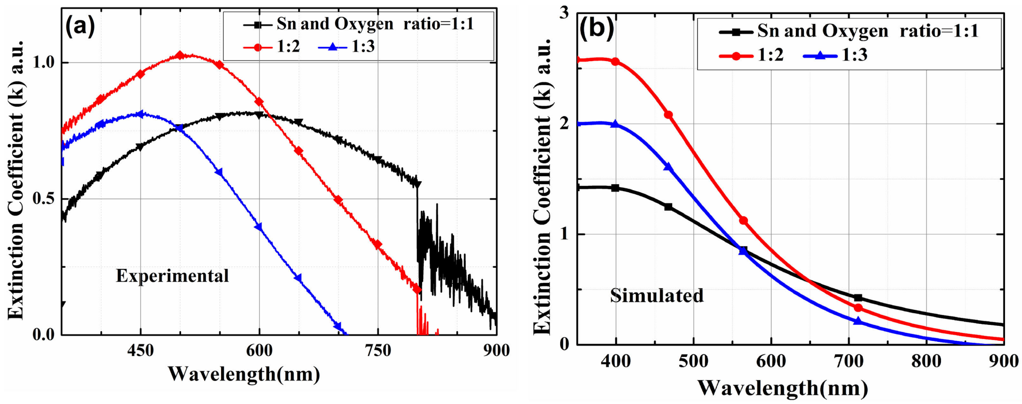


FIGURE 4. Extinction coefficient (k) of SnO films for its different tin and oxygen compositional ratios: (a) experimental and (b) simulated.

of variation in extinction coefficient is somewhat different. The SnO film having the Sn:O ratio as 1:2 shows the highest extinction coefficient as compared to other two ratios of SnO.

The bandgaps obtained from DFT results of SnO film is shown in Fig. 5(a-c) shows that with an increase in Sn:O ratio, i.e., relative increase in amount of oxygen atoms with respect to Sn atoms in SnO crystal, the bandgap of SnO increases with an increase in Sn:O compositional ratio. Figure 5(a) denotes the band gap of SnO film obtained using CASTEP toolkit package of material studio for Sn:O compositional ratio as 1:1, Figure 5(b) represents the bandgap of SnO film for Sn:O compositional ratio as 1:2 and Figure 5(c) shows the band gap of SnO film for Sn:O compositional ratio as 1:3. Experimentally, the band gap in a semiconductor, which corresponds to indirect (non-zero momentum) transitions, can be determined using absorption characteristics by using the Tauc Method which can be expressed as Eq. 3 [19], [20].

$$(\alpha h\nu)^2 = B(h\nu - E_g) \tag{3}$$

where hν is the photon energy, α is the absorption coefficient and B is constant that depends on material. Band gaps are obtained by extrapolating the linear region of the $(\alpha \text{ h } \nu)^2$ versus hν plot to intercept hν-axis to get the direct band gap value [21]. In order to get the indirect band gap value, linear region of $(\alpha \text{ h } \nu)^{1/2}$ versus hν plot are extrapolated to intercept the hν-axis. Band gap of SnO films for its different tin and oxygen ratio have been extracted by Tauc plot as shown in the figure 6 (b). From figure, it is observed that band gap increases with an increase in the Sn:O ratio, which is mainly due to the fact that with an increase in oxygen ratio of SnO film, its properties highly tends to toward the SnO_2 (Tin-dioxide) nature [12], [22], [23].

Figure 6(a) shows the transmittance of SnO film obtained experimentally for Sn:O compositional ratio as 1:1,1:2 and 1:3 using UV-VIS-NIR spectrophotometer. As seen from the Figure 6(a), it is observed that transmittance of SnO film increases with an increase in wavelength of light. Since at higher wavelength, energy of photons or light are much lower than the bandgap value of SnO films, theretofore they are not absorbed at this higher wavelengths and thus transmitted through SnO films. Figure 6(b) represents the band gap values based on experimental data using Tauc plot of SnO film for its different Sn:O compositional ratio as 1:1, 1:2 and 1:3.

We extended the experimental study further to investigate the electrical parameters of SnO films for its different composition of Sn and O ratios using Hall measurement in order to find out nature of SnO films, its carrier concentration, Hall mobility and sheet resistivity using equations given below. The Eq. 4 represents the formula for calculation Hall coefficient, Eq. 5 represents the formula for calculation of carrier concentration and Eq. 6 represents the formula for calculation of Hall mobility.

$$R_H = \frac{(d * V_H)}{(I * B)} \tag{4}$$

$$p = \frac{1}{(R_H * q)} \tag{5}$$

$$\mu_h = (\frac{R_H}{q}) \tag{6}$$

The resistivity of SnO films is given by Eq.7.

$$\rho = R_s * d \tag{7}$$

where ρ is resistivity of SnO film, d is the thickness of SnO films coating on glass substrate. R_S is sheet resistance of SnO films. It is important to note that all the experimentally grown SnO films shows p-type nature. The hole carrier concentration SnO films were obtained to be 9.6 x 10^{18} cm^{-3}, 4.3 x 10^{18} cm^{-3}, 2.4 x 10^{17} cm^{-3}, respectively. It is observed that hole carriers concentration in SnO films reduces as the oxygen ratio, i.e., Sn:O ratio, increases. This is mostly owing to the fact that the oxidation process in SnO films is proportionately improved with an increase in oxygen mole fraction, resulting in the development of a greater number of SnO_2 phases than SnO. One of the key reasons for reduced hole concentration would be insufficient availability of SnO phase at higher growth-O2 condition. The acquired carrier concentration values (10^{17} - 10^{18} cm^{-3}) of SnO films produced under various growth-O_2 conditions accord well with previously published values [8], [9]. However, Hall mobility of a SnO films, increases with an increase in Sn:O ratio.

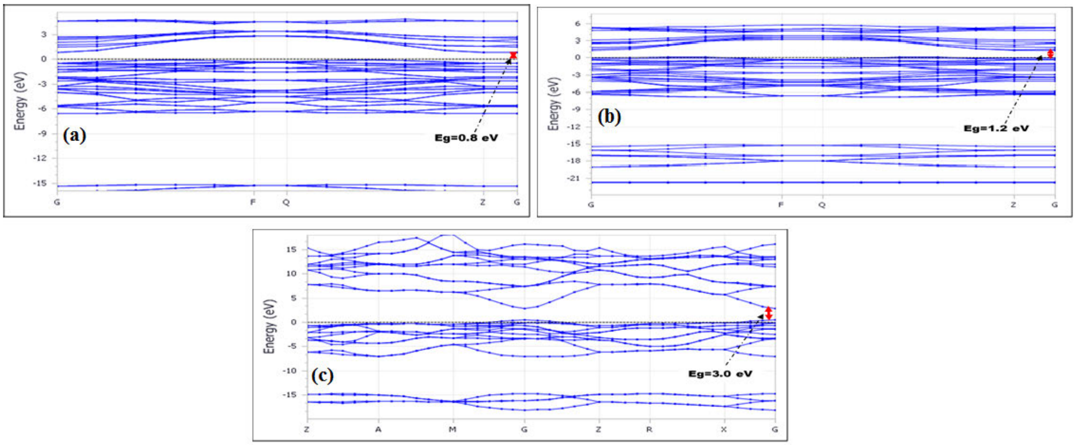


FIGURE 5. (a-c) Band gap of SnO films obtained from DFT simulation for its different tin and oxygen composition ratio.

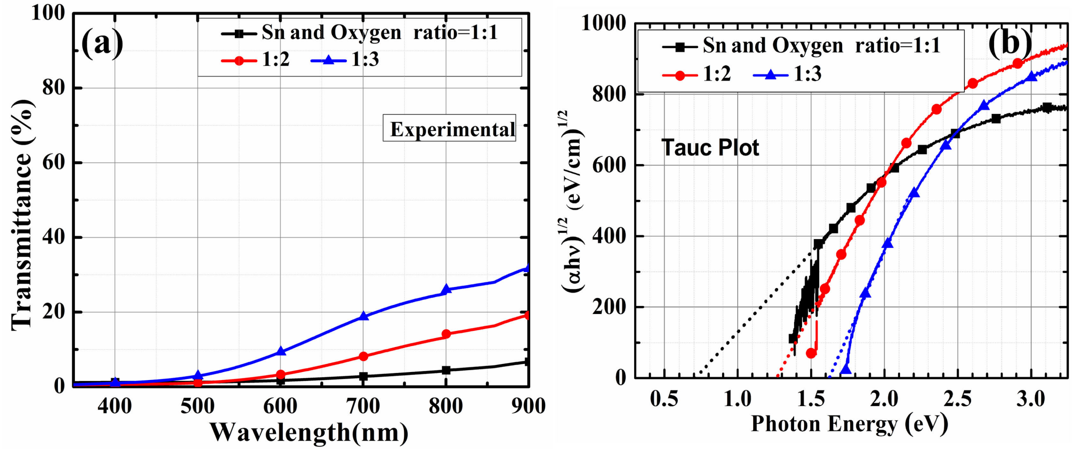


FIGURE 6. (a) Transmittance of SnO films obtained experimentally (b) Band gap extraction of SnO films using Tauc plot for its different tin and oxygen composition ratio..

TABLE 1. Some important parameters of SnO samples obtained using Hall measurement.

Types of SnO samples having different Sn:O ratio	Nature of SnO samples	Hall mobility of SnO samples (cm^3/Vs)	Hole carrier concentration of SnO samples (cm^{-3})	Sheet Resistivity of SnO samples (Ω-cm)
1:1	p-type	6.3	9.6×10^{18}	$8.8{\times}10^{-4}$
1:2	p-type	8.2	4.3×10^{18}	$2.9{\times}10^{-3}$
1:3	p-type	11.2	2.4×10^{17}	$5.8{\times}10^{-3}$

This is mostly due to the previously indicated results which shows a decrement in carrier (hole) concentration with higher growth-O_2 condition. In general, Hall mobility and carrier concentration have an inverse relationship in a semiconductor resulting in a trade-off between hole concentration and Hall mobility of SnO films grown at varied growth-O_2 conditions [24], [25]. Consequently, the resistivity of SnO films were obtained to be 8.8×10^{-4} Ω-cm, 2.9×10^{-3} Ω -cm, and 5.8×10^{-3} Ω-cm.

The Hall measurement of SnO films for its different compositional Sn:O ratios have been tabulated in Table 1 as ready references.

V. CONCLUSION

This work can be concluded by stating that sufficient light absorption property or extinction coefficient in the visible range of solar spectrum and possibility of band gap engineering of SnO film may be a good choice of material for photosensitive devices. The theoretical and experimental trends related to its bandgaps and extinction coefficient are in good agreement with each other. Thus, SnO films of desired characteristics for its use as good material for photosensitive devices can be developed using e-beam evaporation technique by controlling the tin and oxygen ratio in SnO film.

REFERENCES

[1] T. Wildsmith, M. S. Hill, A. L. Johnson, A. J. Kingsley, and K. C. Molloy, "Exclusive formation of SnO by low temperature single-source AACVD," *Chem. Commun.*, vol. 49, no. 78, p. 8773, 2013, doi: 10.1039/c3cc45676e.

[2] Y. Jeon, D. Lee, and H. Yoo, "Recent advances in metal-oxide thin-film transistors: Flexible/stretchable devices, integrated circuits, biosensors, and neuromorphic applications," *Coatings*, vol. 12, no. 2, p. 204, Feb. 2022.

[3] Y. Wang, S. Bruyère, Y. Kumagai, N. Tsunoda, F. Oba, J. Ghanbaja, H. Sun, B. Dai, and J.-F. Pierson, "Tuning the optical band gap and electrical properties of NiO thin films by nitrogen doping: A joint experimental and theoretical study," *RSC Adv.*, vol. 12, no. 34, pp. 21940–21945, Aug. 2022.

[4] S. Ruhle, A. Y. Anderson, H.-N. Barad, B. Kupfer, Y. Bouhadana, E. Rosh-Hodesh, and A. Zaban, "All-oxide photovoltaics," *J. Phys. Chem. Lett.*, vol. 3, no. 24, pp. 3755–3764, Dec. 2012, doi: 10.1021/jz3017039.

[5] P. Qin, Q. He, D. Ouyang, G. Fang, W. C. H. Choy, and G. Li, "Transition metal oxides as hole-transporting materials in organic semiconductor and hybrid perovskite based solar cells," *Sci. China Chem.*, vol. 60, no. 4, pp. 472–489, Apr. 2017, doi: 10.1007/s11426-016-9023-5.

[6] G. K. Dalapati, H. Sharma, A. Guchhait, N. Chakrabarty, P. Bamola, Q. Liu, G. Saianand, A. M. S. Krishna, S. Mukhopadhyay, A. Dey, and T. K. S. Wong, "Tin oxide for optoelectronic, photovoltaic and energy storage devices: A review," *J. Mater. Chem. A*, vol. 9, no. 31, pp. 16621–16684, Aug. 2021, doi: 10.1039/D1TA01291F.

[7] F. C. Sentanin, A. Pawlicka, and C. O. Avellaneda, "Optical and electrochemical properties of SnO_2:Sb thin films prepared by the sol-gel process," *Mol. Cryst. Liq. Cryst.*, vol. 447, no. 1, pp. 243–250, May 2006, doi: 10.1080/15421400500377263.

[8] A. M. Ganose and D. O. Scanlon, "Band gap and work function tailoring of SnO_2 for improved transparent conducting ability in photovoltaics," *J. Mater. Chem. C*, vol. 4, no. 7, pp. 1467–1475, 2016, doi: 10.1039/C5TC04089B.

[9] Y. Ogo, H. Hiramatsu, K. Nomura, H. Yanagi, T. Kamiya, M. Kimura, M. Hirano, and H. Hosono, "Tin monoxide as an S-orbital-based P-type oxide semiconductor: Electronic structures and TFT application," *Phys. Status Solidi A, Appl. Mater. Sci.*, vol. 206, no. 9, pp. 2187–2191, Jul. 2009, doi: 10.1002/pssa.200881792.

[10] D. E. Guzmán-Caballero, M. A. Quevedo-López, and R. Ramírez-Bon, "Optical properties of P-type SnO_x thin films deposited by DC reactive sputtering," *J. Mater. Sci., Mater. Electron.*, vol. 30, no. 2, pp. 1366–1373, Jan. 2019, doi: 10.1007/s10854-018-0406-1.

[11] W. Guo, L. Fu, Y. Zhang, K. Zhang, L. Y. Liang, Z. M. Liu, H. T. Cao, and X. Q. Pan, "Microstructure, optical, and electrical properties of P-type SnO thin films," *Appl. Phys. Lett.*, vol. 96, no. 4, Jan. 2010, Art. no. 042113, doi: 10.1063/1.3277153.

[12] M. Kumar, S. S. A. Askari, and M. K. Das, "Oxygen controlled E-beam evaporation deposited p-SnO_x thin film for photosensitive devices," *Mater. Lett.*, vol. 257, Dec. 2019, Art. no. 126684, doi: 10.1016/j.matlet.2019.126684.

[13] J. Gupta, P. A. Hassan, and K. C. Barick, "Defects in nanomaterials for visible light photocatalysis," in *Nanostructured Materials for Visible Light Photocatalysis*. Amsterdam, The Netherlands: Elsevier, 2022, pp. 319–350.

[14] S. Jiang, Y. Li, Z. Chen, W. Zhu, Q. Wu, H. He, and X. Wang, "The effects of defects on the defect formation energy, electronic band structure, and electron mobility in 4H–SiC," *AIP Adv.*, vol. 12, no. 6, Jun. 2022, Art. no. 065311.

[15] L. Grzadziel, M. Krzywiecki, A. Szwajca, A. Sarfraz, G. Genchev, and A. Erbe, "Detection of intra-band gap defects states in spin-coated sol-gel SnO_x nanolayers by photoelectron spectroscopies," *J. Phys. D, Appl. Phys.*, vol. 51, no. 31, Aug. 2018, Art. no. 315301.

[16] A. Verma, U. Kumar, P. Chaudhary, and B. C. Yadav, "Investigation on structural and optical properties of porous SnO_2 nanomaterial fabricated by direct liquid injection chemical vapour deposition technique," *Solid State Commun.*, vols. 348–349, Jun. 2022, Art. no. 114723, doi: 10.1016/j.ssc.2022.114723.

[17] B. Adamowicz, W. Izydorczyk, J. Izydorczyk, A. Klimasek, W. Jakubik, and J. Zywicki, "Response to oxygen and chemical properties of SnO_2 thin-film gas sensors," *Vacuum*, vol. 82, no. 10, pp. 966–970, Jun. 2008, doi: 10.1016/j.vacuum.2008.01.003.

[18] A. A. Abozeed, O. Younis, A. F. Al-Hossainy, N. A. El-Mawla, M. Sayed, A. M. K. El-dean, and M. S. Tolba, "Combined experimental and TD-DFT/$DMOl_3$ investigations, optical properties, and photoluminescence behavior of a thiazolopyrimidine derivative," *Sci. Rep.*, vol. 12, no. 1, p. 15674, Sep. 2022, doi: 10.1038/s41598-022-19840-y.

[19] J. Tauc, "Optical properties and electronic structure of amorphous Ge and Si," *Mater. Res. Bull.*, vol. 3, no. 1, pp. 37–46, 1968, doi: 10.1016/0025-5408(68)90023-8.

[20] J. Tauc, R. Grigorovici, and A. Vancu, "Optical properties and electronic structure of amorphous germanium," *Phys. Status Solidi B*, vol. 15, no. 2, pp. 627–637, 1966, doi: 10.1002/pssb.19660150224.

[21] A. S. Hassanien and A. A. Akl, "Influence of composition on optical and dispersion parameters of thermally evaporated non-crystalline $Cd_{50}S_{50-x}Se_x$ thin films," *J. Alloys Compounds*, vol. 648, pp. 280–290, Nov. 2015, doi: 10.1016/j.jallcom.2015.06.231.

[22] H. I. Bang, H. B. Seo, B. S. Bae, and E. Yun, "Effects of oxygen ratio on the properties of tin oxide thin films doped with bismuth," *Phys. Status Solidi (A)*, vol. 216, no. 9, May 2019, Art. no. 1800863, doi: 10.1002/pssa.201800863.

[23] M. Sun, Z. Gong, H. Yin, Z. Zhang, Y. Li, H. Dong, W. Jing, D. Xie, H. Liang, and F. Wu, "Competition and cooperation between fluorine and oxygen in SnO_2:F films," *Crystals*, vol. 11, no. 8, p. 873, Jul. 2021, doi: 10.3390/cryst11080873.

[24] J. T. Wang, X. L. Shi, W. W. Liu, X. H. Zhong, J. N. Wang, L. Pyrah, K. D. Sanderson, P. M. Ramsey, M. Hirata, and K. Tsuri, "Influence of preferred orientation on the electrical conductivity of fluorine-doped tin oxide films," *Sci. Rep.*, vol. 4, no. 1, p. 3679, Jan. 2014, doi: 10.1038/srep03679.

[25] Y. Peng, L. Miao, J. Gao, C. Liu, M. Kurosawa, O. Nakatsuka, and S. Zaima, "Realizing high thermoelectric performance at ambient temperature by ternary alloying in polycrystalline $Si_{1-x-y}Ge_xSn_y$ thin films with boron ion implantation," *Sci. Rep.*, vol. 9, no. 1, p. 14342, Oct. 2019, doi: 10.1038/s41598-019-50754-4.

[26] M. El-Hagary, M. Emam-Ismail, E. R. Shaaban, and A. El-Taher, "Effect of γ-irradiation exposure on optical properties of chalcogenide glasses $Se_{70}S_{30-x}Sb_x$ thin films," *Radiat. Phys. Chem.*, vol. 81, no. 10, pp. 1572–1577, Oct. 2012.

[27] J. Wang, H. Li, S. Meng, X. Ye, X. Fu, and S. Chen, "Controlled synthesis of Sn-based oxides via a hydrothermal method and their visible light photocatalytic performances," *RSC Adv.*, vol. 7, no. 43, pp. 27024–27032, 2017.

[28] S. Qiu, Z. Lin, Y. Zhou, D. Wang, L. Yuan, Y. Wei, T. Dai, L. Luo, and G. Chen, "Highly selective colorimetric bacteria sensing based on protein-capped nanoparticles," *Analyst*, vol. 140, no. 4, pp. 1149–1154, 2015.

[29] C. M. Campo, J. E. Rodríguez, and A. E. Ramírez, "Thermal behaviour of romarchite phase SnO in different atmospheres: A hypothesis about the phase transformation," *Heliyon*, vol. 2, no. 5, May 2016, Art. no. e00112.

[30] H. Ilchuk, R. Petrus, A. Kashuba, I. Semkiv, and E. Zmiiovska, "Optical-energy properties of CdSe thin film," *Mol. Cryst. Liq. Cryst.*, vol. 699, no. 1, pp. 1–8, 2020.

MANOJ KUMAR received the Ph.D. degree from the Department of Electronics Engineering, IIT (ISM) Dhanbad, India. He has worked as a Junior Research Fellow with the Department of Electronics Engineering, IIT (ISM) Dhanbad. He is currently an Assistant Professor with the MLR Institute of Technology, Hyderabad, India. His current research interests include the growth and development of metal-oxide-based optoelectronic devices, such as thin-film solar cells and sensors.

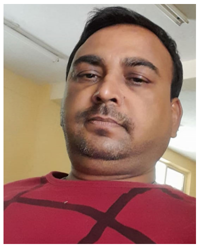
SYED SADIQUE ANWER ASKARI received the Ph.D. degree from the Department of Electronics Engineering, IIT (ISM) Dhanbad, India. From 2013 to 2014, he worked as a Junior Research Fellow with the Department of Electronics and Electrical Communication Engineering, IIT Kharagpur, India. He is currently a Research Associate with the Centre of Excellence in Renewable Energy, IIT (ISM) Dhanbad. His current research interest includes sustainable efficiency improvement of oxide-based photovoltaic devices, especially on metal–oxide/Si heterojunction solar cells.

PURNENDU SHEKHAR PANDEY (Senior Member, IEEE) received the Ph.D. degree from the Indian Institute of Technology (Indian School of Mines) Dhanbad, India. He has worked as a Junior Research Fellow in the Indian Space Research Organization (ISRO)-sponsored project (Sanction No. ISRO/RES/3/775/18-19) with the Indian Institute of Technology (Indian School of Mines) Dhanbad. He is currently an Assistant Professor with the Department of Electronics and Communication Engineering, GL Bajaj Institute of Technology and Management, Greater Noida, India. He has more than 10 years of experience in academics and research. He has also authored a textbook titled *Power Line Carrier Communication and Arduino Based Automation* (Research India Publication, 2017). He has published more than 55 high-quality research papers in national and international SCI journals and conferences. He holds eight published patents and one granted patent. His current research interests include optical sensors, nano and biophotonics, photonic and plasmonic devices, wireless sensor networks, and biomedical engineering. He is a member of SPIE.

YADVENDRA SINGH (Member, IEEE) received the Ph.D. degree in fiber optic sensors from the Department of Electronics Engineering, Indian Institute of Technology (Indian School of Mines) Dhanbad, India. He is currently a Postdoctoral Researcher with the School of Electrical Engineering and Computer Science, Oregon State University, Corvallis, OR, USA. His current research interests include designing passive, integrated devices using waveguides, and fiber optic-based plasmonic sensors. He is a member of OSA, SPIE, and OSI.

RAJESH SINGH (Member, IEEE) received the B.E. degree (Hons.) from Dr. B. R. Ambedkar University, Agra, Uttar Pradesh, India, and the M.Tech. degree (Hons.) from RGPV, Bhopal, Madhya Pradesh, India. He is currently a Professor with Uttaranchal Institute of Technology, Uttaranchal University, Dehradun, India, with more than 18 years of experience in academics. His research interests include embedded systems, robotics, wireless sensor networks, the Internet of Things, and machine learning. He has been awarded a gold medal for the M.Tech. degree from RGPV. He has been honored as a keynote speaker and the session chair of international/national conferences, faculty development programs, workshops, and webinars. He has 358 patents filed, including 13 patents granted (eight Australian and five Indian patents) and five PCT. He has published more than 100 research papers in refereed journals/conferences. He has published 24 authored and seven edited books in the areas of embedded systems and the Internet of Things with reputed publishers, such as CRC/Taylor & Francis, Springer, Narosa, NIPA, River Publishers, Bentham Science, IGI Global, and NOVA Science. He has been featured by Indian and international media for the smart systems and devices designed by him, including OBDAS, E-Parirakshak, Kawach, 20Sec4Life, Ally, Alithis, CT scan diagnosis, among which five are designed to prevent COVID-19, as per WHO guidelines.

SANJEEV KUMAR RAGHUWANSHI (Senior Member, IEEE) received the bachelor's degree in electronic and instrumentation engineering from Shri Govindram Seksaria Institute of Technology and Science, Indore, Madhya Pradesh, India, in August 1999, the master's degree in solid state technology from IIT Kharagpur, Kharagpur, India, in January 2002, and the Ph.D. degree in the field of optics from the Department of Electrical Communication Engineering. He worked as a Postdoctoral Research Fellow with the Instrumentation and Sensor Division, School of Engineering and Mathematical Sciences, City University of London, London, U.K., from 2014 to 2015. He is currently an Associate Professor with the Department of Electronics Engineering, IIT (ISM) Dhanbad. In the previous ten years, he has published over 100 peer-reviewed and indexed international SCI journal articles. He has published six books in the field of current optical fibers. Six Indian patents have been filed and published by him in the last five years. He was awarded the Erusmus Mundus Scholarship for the Ph.D. degree. He has contributed to IEEE Transactions on Instrumentation and Measurement, IEEE Sensors Journal, IEEE Photonics Technology Letters, and IEEE Journal of Quantum Electronics, as a Reviewer. He serves as a reviewer on the editorial boards for various Indian publications. He has been awarded the Best Research Award (Canara Bank Publication Award) by the Indian Institute of Technology (ISM) Dhanbad, in 2016, 2017, and 2018.



GYANENDRA KUMAR SINGH received the Ph.D. degree in mechanical engineering from the Motilal Nehru National Institute of Technology Allahabad, Prayagraj, India, (an Institute of National Importance), in 2011. He is currently an Associate Professor with Adama Science and Technology University, Adama, Ethiopia. He has over two decades of experience in academics and research. He has published more than 50 articles in reputed journals. He holds a Lifetime Membership of the Indian Society of Technical Education. His research interests include the interdisciplinary field of computer science (the IoT and deep learning), material science, but are not limited to smart materials, such as 4-D printed materials, self-healing composites, and bio functional nanofibers, and the modeling and optimization of modern manufacturing processes.

SANTOSH KUMAR (Senior Member, IEEE) received the Ph.D. degree from the Indian Institute of Technology (Indian School of Mines) Dhanbad, Dhanbad, India. He is currently an Associate Professor with the School of Physics Science and Information Technology, Liaocheng University, Liaocheng, China. His current research interests include optical fiber sensors, nano and biophotonics, photonic and plasmonic devices, and waveguides and interferometers. He has supervised 12 M.Tech. dissertations and six Ph.D. candidates. He has published more than 270 high-quality research articles in national and international SCI journals and conferences. He has presented numerous papers at conferences held in China, India, Belgium, and USA. He has recently published two scholarly books, titled *2D Materials for Surface Plasmon Resonance-Based Sensors* (CRC Press, 2021) and *Optical Fiber-Based Plasmonic Biosensors: Trends, Techniques, and Applications* (CRC Press, 2022). He has also authored a textbook titled *Fiber Optic Communication: Optical Waveguides, Devices, and Applications* (University Press, 2017). He has reviewed over 1500 SCI journals published by IEEE, Elsevier, Springer, OPTICA, SPIE, Wiley, and Nature, up to this point. He has been a Senior Member of OPTICA and a Fellow Member of SPIE, since 2023. He is also an OPTICA Traveling Lecturer. He has received the "2022 Best Performing Associate Editor" Award from IEEE Sensors Journal. He is also the Chair of the OPTICA Optical Biosensors Technical Group. He has given numerous invited speeches and serves as the session chair for IEEE conferences. He serves as an Associate Editor for IEEE Sensors Journal, IEEE Access, IEEE Transactions on NanoBioscience, *Frontiers of Physics*, and *Biomedical Optics Express*.