INVESTIGATION OF ENERGY BAND GAP OF Sb DOPED SnO_2 THIN FILMS

Zin Mar Win[1], Ohn Mar Swe[2], Amy Than[3] and Moht Moht Than[4]

Abstract

Undoped SnO_2 and different Sb concentration (2 mol%, 4 mol%, 6 mol% & 8 mol%) were doped with SnO_2 thin films by sol-gel process. *Undoped SnO_2* and *Sb doped SnO_2 thin films* were grown in glass substrate by using spin coating technique and annealed at 500˚C for 1hour. The structural, and optical properties of deposited and doped samples were studied. XRD analysis was carried out to determine the lattice parameters, unit cell volume and *crystallite size* of the samples. According to the X-ray diffraction spectra the samples were formed with tetragonal structure and preferred orientation alone (110) plane. The dislocation density of the samples are also calculated. From the UV-Visible spectrum, absorption coefficient and the *band gap energy* of the samples are evaluated.

Keywords: Undoped SnO_2 and Sb doped SnO_2 thin films, crystallite size, and band gap energy

Introduction

Semiconductors are one of the most interesting and most useful solids. They have been investigated many times because of their flexibility, electricity and optical features.SnO_2 is one of these semiconductors. The SnO_2 with a wide-band-gap (E_g = 3.6 ~ 4.0 eV) is one of the excellent semiconductors which can be applied to solid state gas sensors, sensing arrays, solar cells, photovoltaic cells, organic light emitting diodes, touch sensitive screens and thin film transistors. [Bagheri Mohaghegi M M et al (2008), Khan AF et al (2010), Moharrami F et al (2012)]. The SnO_2 thin films can be fabricated by a number of techniques such as chemical vapour deposition (CVD), metalorganic deposition, rf sputtering, sol-gel dip coating, spin coating and spray pyrolysis. [Maekava T et al (2001), Yin LT et al (2000), Yin LT et al (2000), Ouerfelli J et al (2008).] It was clearly established spin coating that structural, electronic transport and optical properties of SnO_2 films are very sensitive to preparation method, deposition conditions, dopant atoms and amount of dopant atoms. Tin dioxide (SnO_2) has been intensively investigated because of its rich physical properties and large applications in commercial devices.

Experimental

The glass substrates were ultrasonically cleaned by keeping in ethanol and in the distilled water, for ten minutes, respectively. Then the glass substrates were dried. The films deposited on the glass substrates by spin coating technique. In order to prepare the coating solution, firstly, undoped SnO_2 and different Sb concentration (2 mol%, 4 mol%, 6 mol% & 8 mol%) were doped with thin films by sol-gel process. The mixture powder is ground by agate mortor to obtain the homogeneous and uniform grain size of powder. This powder is heat treated at 500ºC for 1 hr. The crystalline powder, were mixed with 2-methoxyethanol solution by using sol-gel method.

[1] Dr, Lecturer, Department of Physics, University of Yangon.
[2] Lecturer, Department of Physics, University of Yangon.
[3] Lecturer, Department of Physics, University of Yangon.
[4] Associate Professor Department of Physics, Mohnyin Degree College.

And then these pastes were coated on glass substrates and annealed at 500ºC for 1 hr, respectively.

Results and Discussion

The structure of prepared films were characterized by X-ray diffraction (Rigaku Multiflex, Japan) with Cu K_α source (λ =1.54056 Å).

The XRD analysis of the as-synthesized undoped SnO_2 and with different concentration of Sb thin films on glass is shown in figure 1 (a ~ e). The diffraction patterns of the samples match the tetragonal structure. Furthermore, increasing the antimony content did not yield any other crystalline phase. The films show a preferred orientation along the (110), (101), (200) and (211) planes. The lattice constants a and c for the tetragonal phase structure are determined by the relation,

$$\frac{1}{d^2}=\left(\frac{h^2}{a^2}+\frac{k^2}{a^2}\right)+\left(\frac{l^2}{c^2}\right)$$

where d and (hkl) are interplanar distance and Miller indices, respectively. The lattice constant a and c, the unit cell volumes are calculated as given in Table 1. They match well with the standard JCPDS data card. In order to determine the variation of crystallite size with increasing Sb doping, the size of the crystallites oriented along the (110) plane is calculated using Scherrer's formula,

$$L=\frac{0.9\lambda}{\beta\cos\theta}$$

where β,θ and λ are the broadening of the diffraction line measured at half its maximum intensity in radians, the diffraction angle, and the X-ray wavelength, respectively. The calculated values of unit cell volume are given in Table 1. Dislocation density and crystallite size are given in Table 2.

Table 1 The structural properties of undoped SnO_2 and Sb doped SnO_2 thin films on glass substrate

Samples	***Maximum peak***	***Lattice constant "a"(Å)***	***Lattice constant "c"(Å)***	***Unit cell volume "V" (nm)^3***
Undoped SnO_2	(110)	4.8365	3.2068	0.0750
Sb (2mol%) doped SnO_2	(110)	4.8138	3.1941	0.0740
Sb (4mol%) doped SnO_2	(110)	4.8609	3.1973	0.0755
Sb (6mol%) doped SnO_2	(110)	4.8024	3.1931	0.0736
Sb (8mol%) doped SnO_2	(110)	4.8519	3.1950	0.0752

Table 2 The values of dislocation density and crystallite size of undoped SnO_2 and Sb doped SnO_2 thin films on glass substrate

Samples	***Maximum peak***	***Crystallite size "L" (nm)***	***Dislocation density "δ" $(m)^{-2}$***
Undoped SnO_2	(110)	61.3222	2.6593×10^{14}
Sb (2 mol%) doped SnO_2	(110)	58.2183	2.9504×10^{14}
Sb (4 mol%) doped SnO_2	(110)	57.8355	2.9896×10^{14}
Sb (6 mol%) doped SnO_2	(110)	55.1036	3.2934×10^{14}
Sb (8 mol%) doped SnO_2	(110)	52.5894	3.6158×10^{14}

The optical transmittance (T%) spectrum of undoped SnO_2 and Sb doped SnO_2 thin films was taken in the wavelength range 300 ~ 1100 nm. Figure 2 (a ~ e) shows the variation of optical transmittance with the wavelength of thin films. The fundamental absorption corresponding to the optical transition of the electrons from the valence band to the conduction band can be used to determine the nature and value of the optical band gap E_g of the films.

The optical absorption coefficient (α) was calculated from transmittance using the following relation,

$$\alpha = \frac{1}{d}\log(\frac{1}{T})$$

where T is the transmittance and d is the thickness of the films. The films under study have an absorption coefficient (α) obeying following relation for high photon energies (hν)

$$\alpha = \frac{A(h\nu - E_g)^{1/2}}{h\nu}$$

where E_g is the optical band gap of the films and A is a constant. A plot of variation of $(\alpha h\nu)^2$ versus hν is shown in Figure 3 (a ~ e). E_g is evaluated using the extrapolation of the linear part. The intercept on energy axis gives the value of band gap energy. Upon increasing the Sb concentration, the band gap of the films was found to increase from 3.43 eV to 4 eV. Optical band gap energy with different Sb doped SnO_2 thin films is shown in Table (3).

Table 3 Optical band gap energy with different Sb doped SnO_2 thin films.

Sb doped SnO_2	**Band gap energy (eV)**
Undoped SnO_2	3.43eV
Sb (2mol%) doped SnO_2	3.85eV
Sb (4mol%) doped SnO_2	3.91eV
Sb (6 mol%) doped SnO_2	3.98eV
Sb (8mol%) doped SnO_2	4 eV

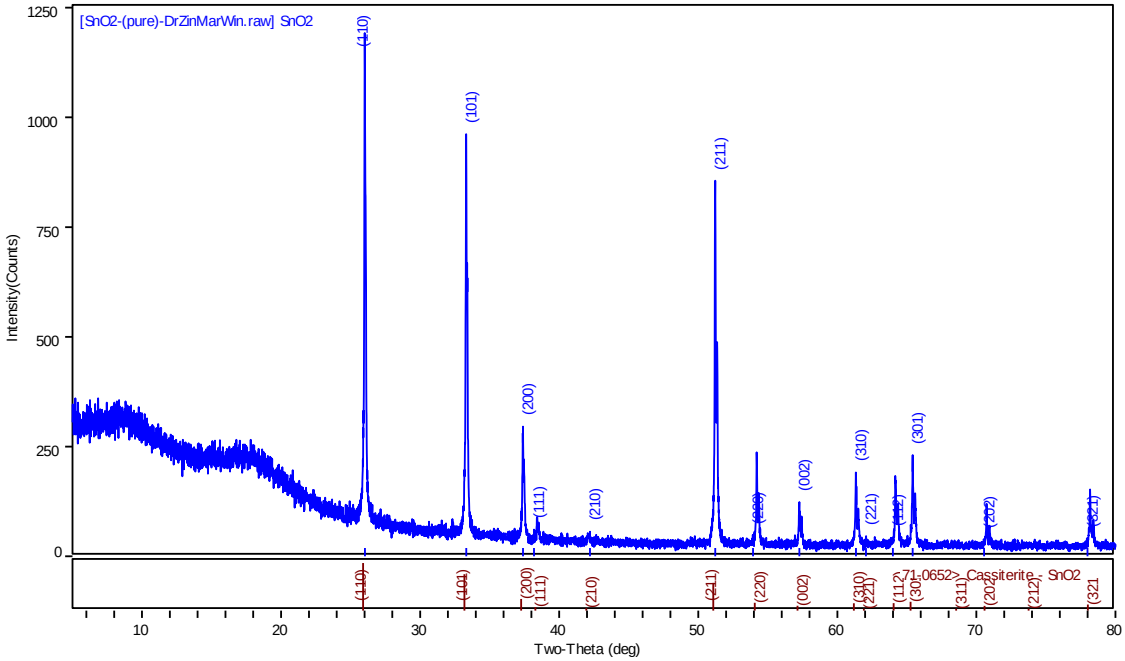

Figure 1 (a) XRD pattern of undoped SnO_2 thin film on glass

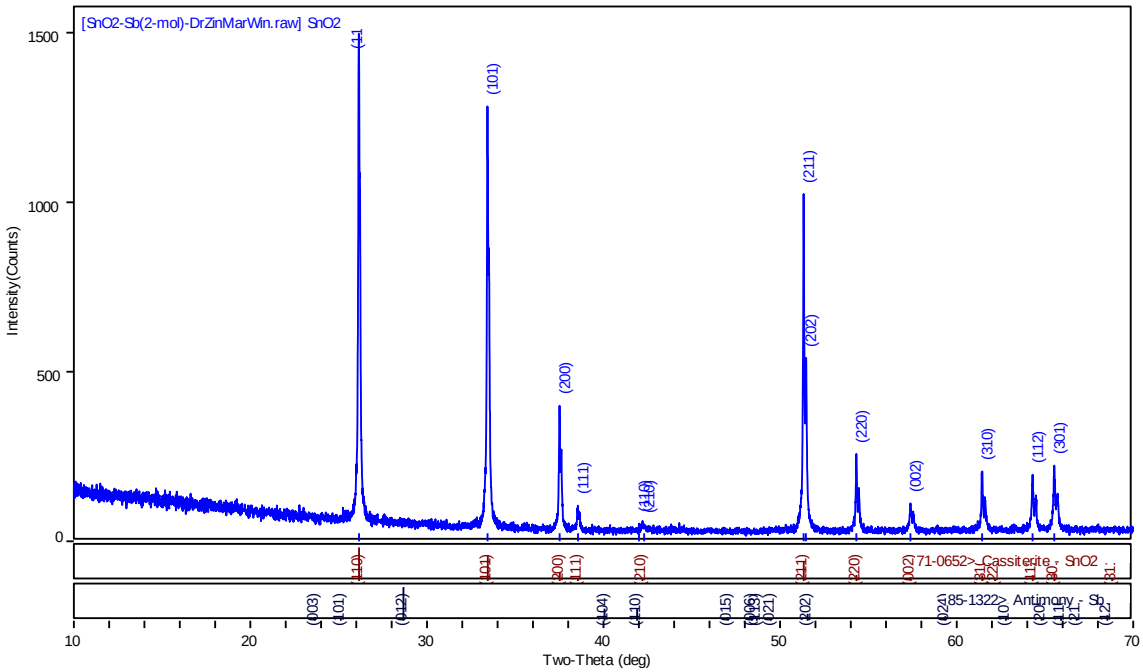

Figure 1 (b) XRD pattern of Sb (2 mol%) doped SnO_2 thin film on glass

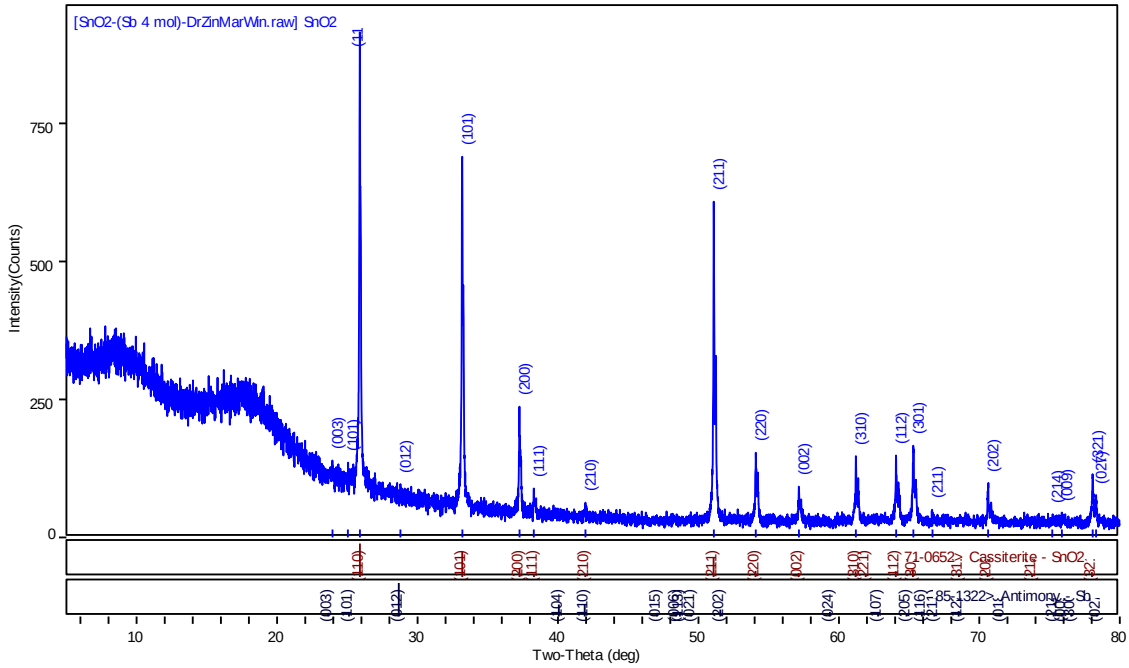

Figure 1 (c) XRD pattern of Sb (4 mol%) doped SnO_2 thin film on glass

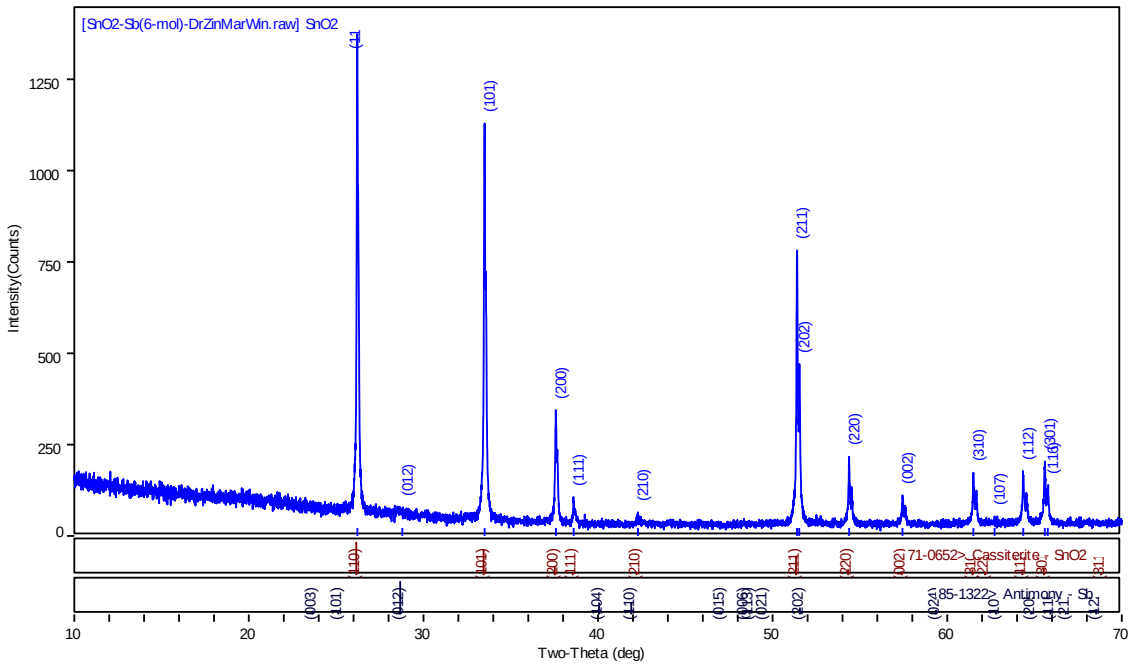

Figure 1 (d) XRD pattern of Sb (6 mol%) doped SnO_2 thin film on glass

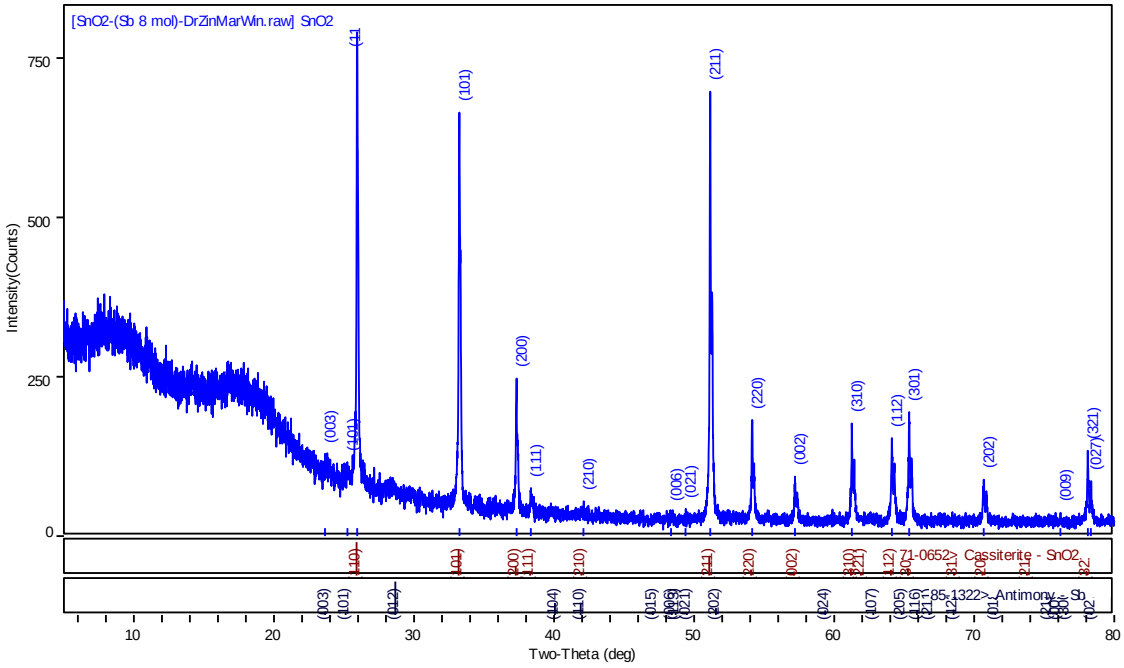

Figure 1 (e) XRD pattern of Sb (8 mol%) doped SnO_2 thin film on glass

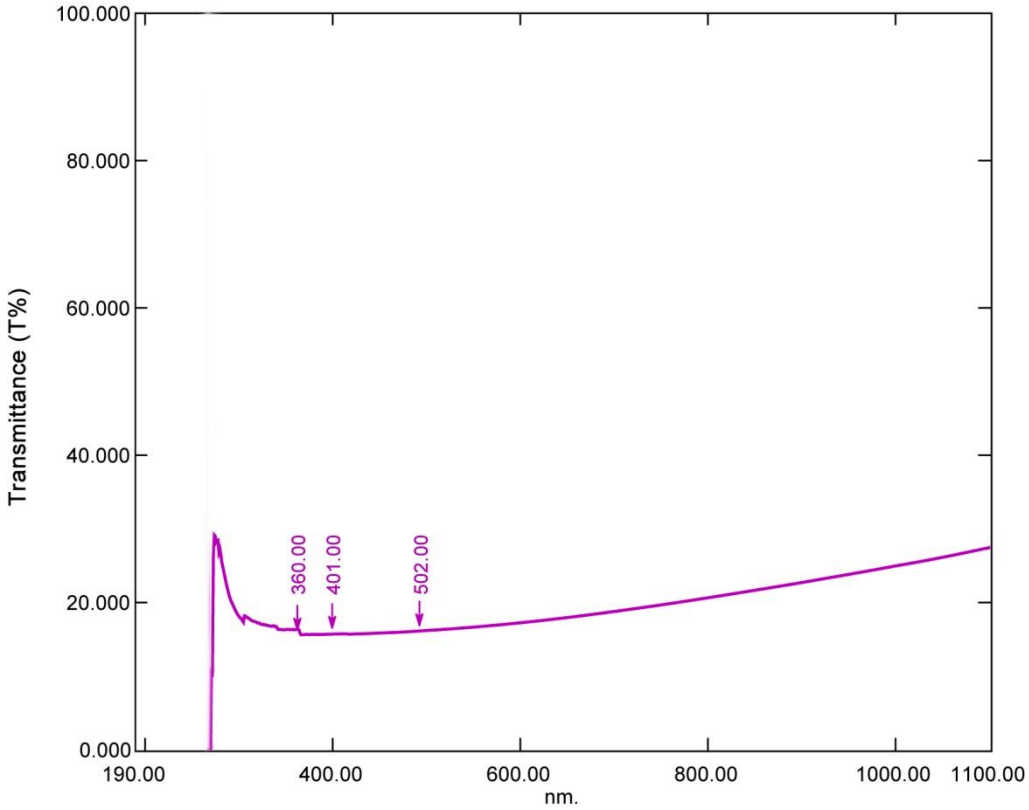

Figure 2 (a) Transmittance (T%) spectra for undoped SnO_2 thin film on glass

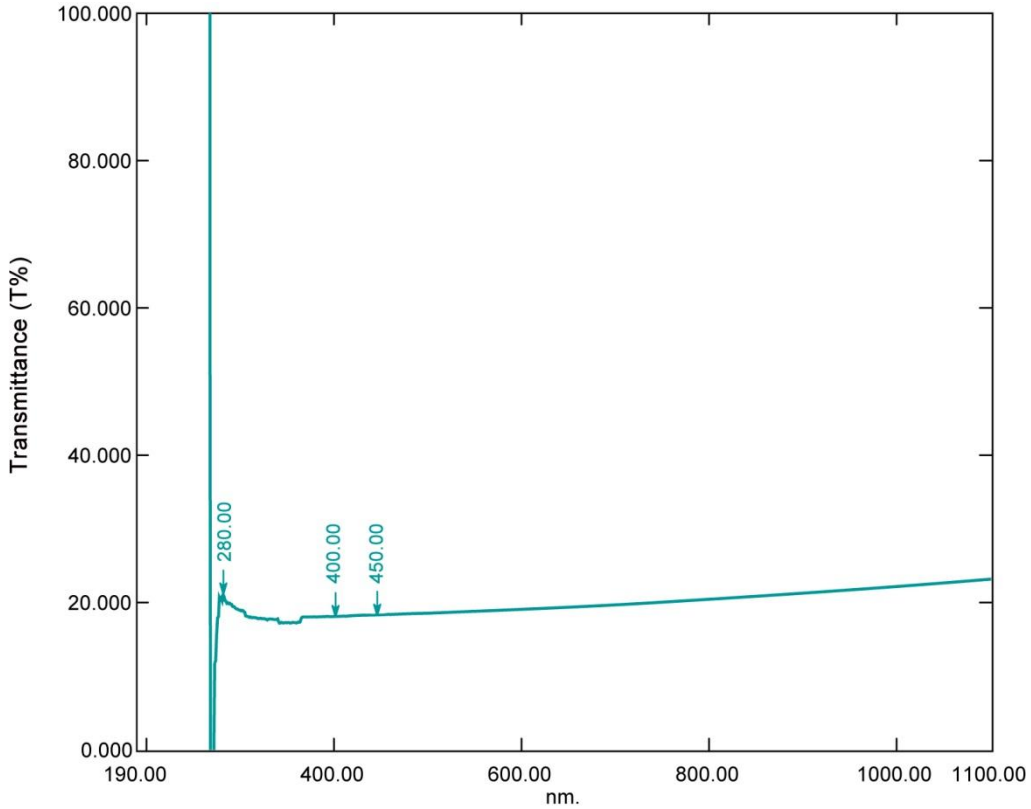

Figure 2 (b) Transmittance (T%) spectra for Sb (2 mol%) doped SnO_2 thin film on glass

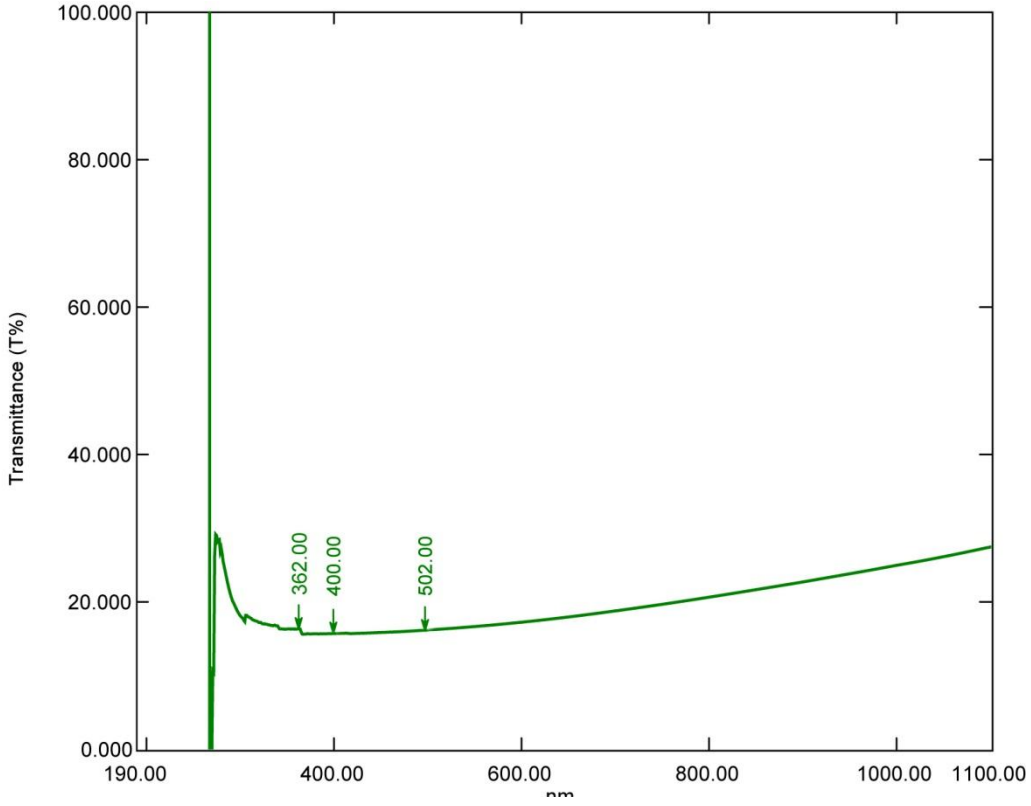

Figure 2 (c) Transmittance (T%) spectra for Sb (4 mol%) doped SnO_2 thin film on glass

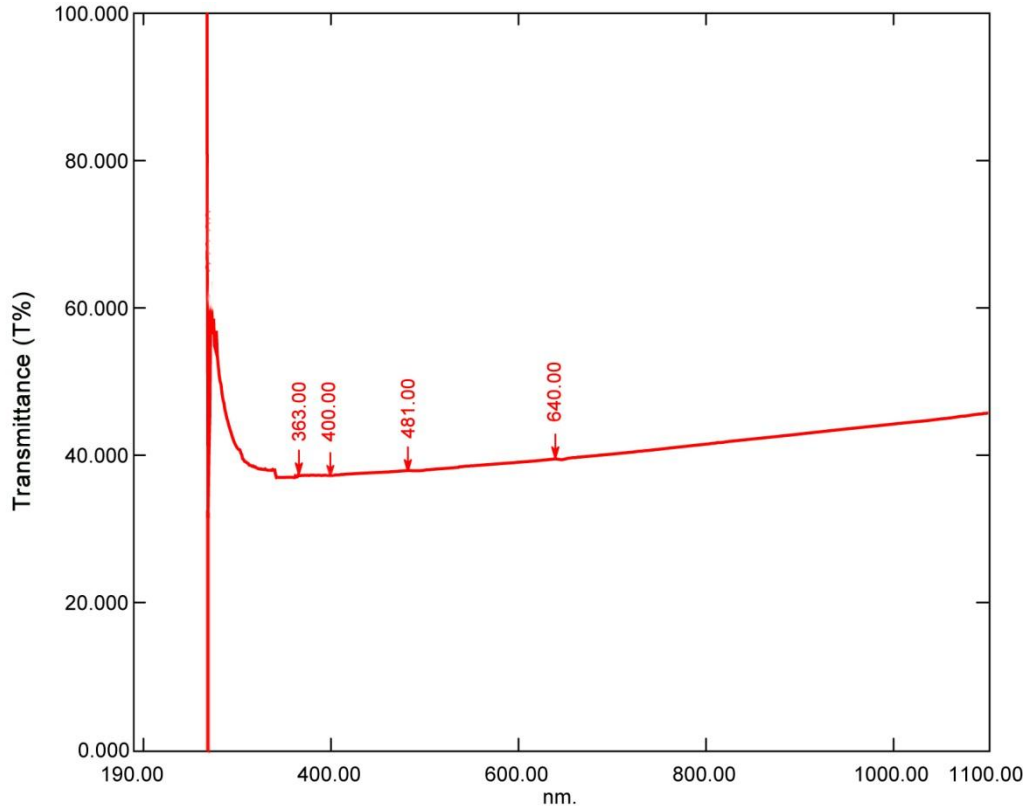

Figure 2 (d) Transmittance (T%) spectra for Sb (6 mol%) doped SnO_2 thin film on glass

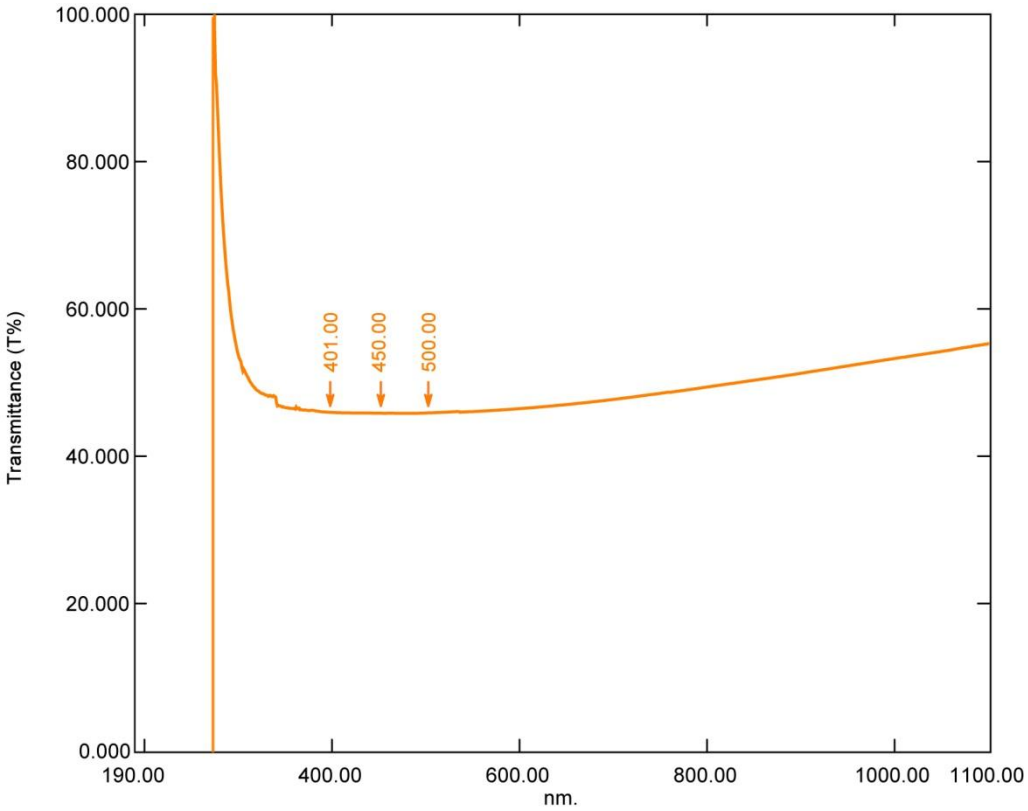

Figure 2 (e) Transmittance (T%) spectra for Sb (8 mol%) doped SnO_2 thin film on glass

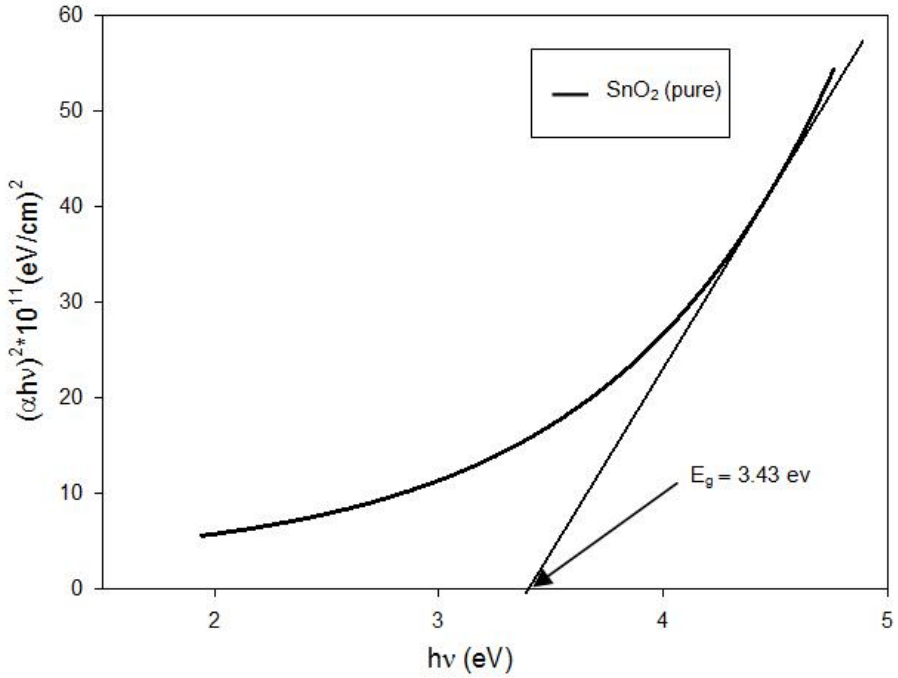

Figure 3 (a) Plot of $(\alpha h\nu)^2$ versus hν (undoped SnO_2)

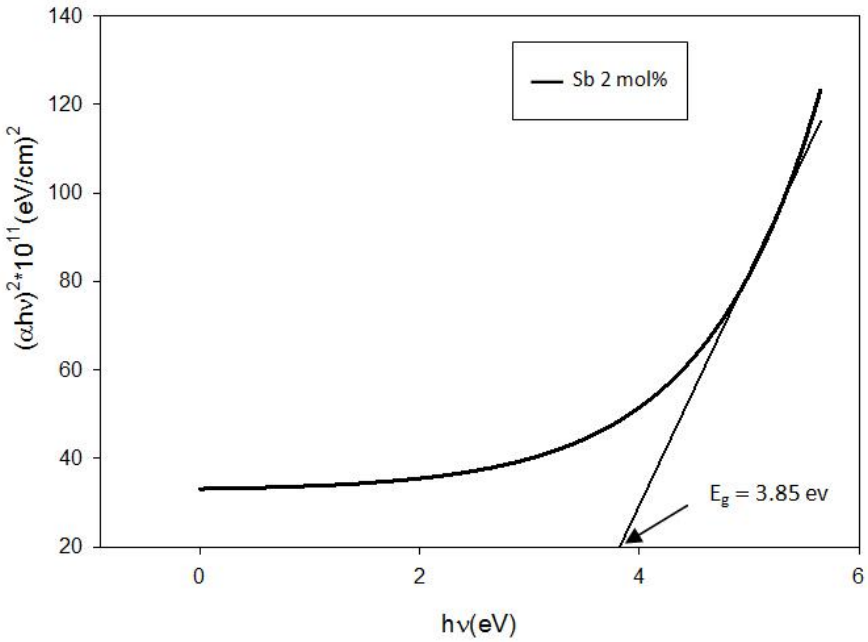

Figure 3 (b) Plot of $(\alpha h\nu)^2$ versus hν (Sb 2 mol% doped)

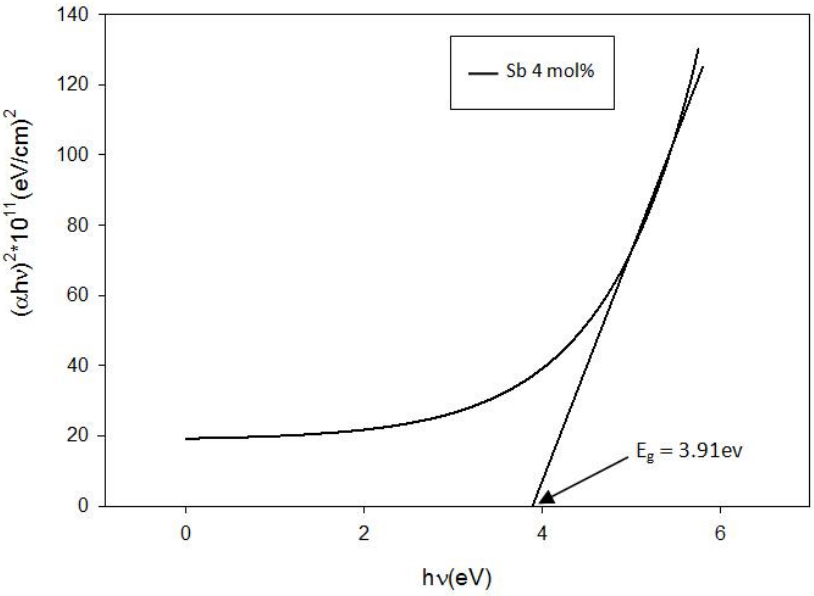

Figure 3 (c) Plot of $(\alpha h\nu)^2$ versus hν (Sb 4 mol% doped)

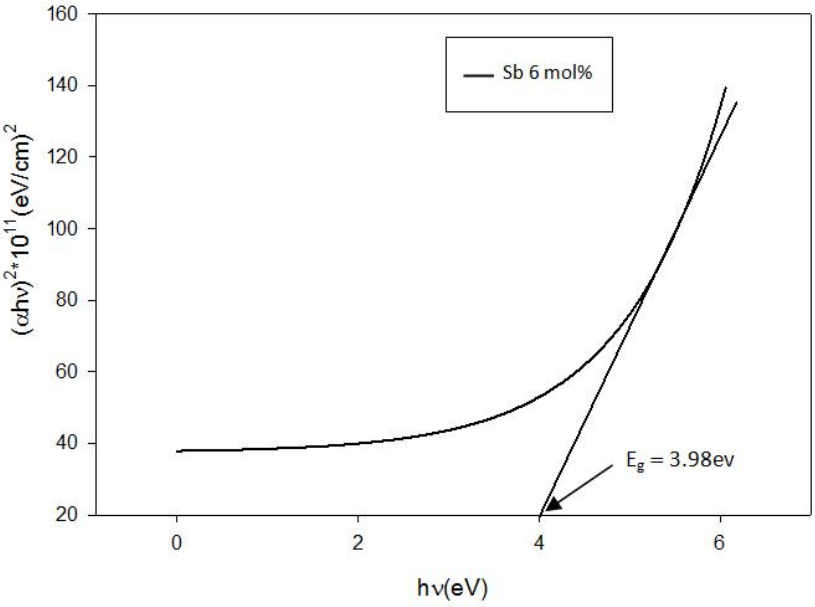

Figure 3 (d) Plot of $(\alpha h\nu)^2$ versus hν (Sb 6 mol% doped)

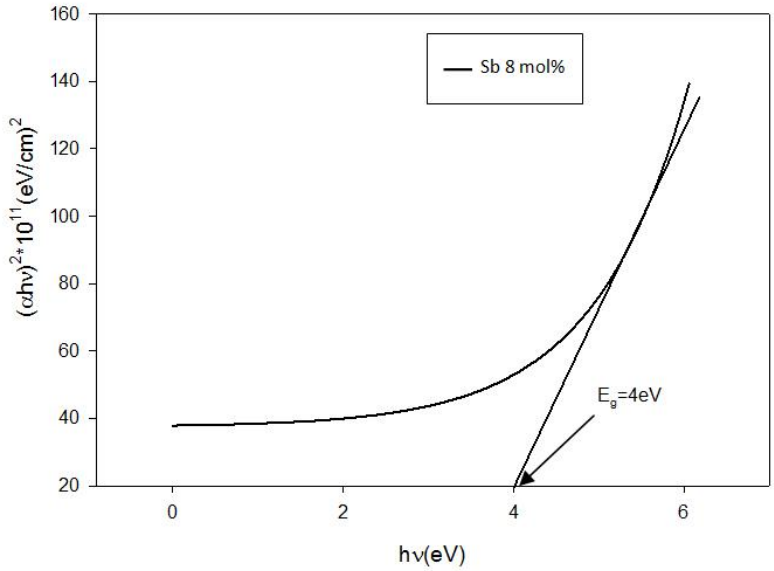

Figure 3 (e) Plot of $(\alpha h\nu)^2$ versus hν (Sb 8 mol% doped)

Conclusion

The undoped SnO_2 and Sb doped SnO_2 thin films on glass were prepared by using sol-gel and spin coating method. The Sb doped concentration changed from 2 mol% to 8 mol%. The X-ray measurements, the lattice constants were a = b= 4.83Å and c = 3.20Å. It was also observed that the different Sb concentration did not change the lattice parameters. The average crystallite size of the samples was in the range 52 ~ 61 nm. The band gap energy of the samples is varied from 3.43 eV to 4 eV. The study of these results shows that the Sb doped SnO_2 thin films can be suitable for optoelectronic applications.

Acknowledgements

I wish to express my sincere thanks to Professor Dr Khin Khin Win, Head of Department of Physics, Yangon University, for her kind permission to carry out this research.

I would like to express my sincere thanks to Dr Myo Lwin, Professor, Dr Ye Chan, Professor and Head, Universities' Research Center, Dr Aye Aye Thant, Professor, Department of Physics, Dr Yin Maung Maung, Professor, Department of Physics and Dr Than Zaw Oo, Professor, Universities' Research Center, University of Yangon, for their suggestion and comments for this work.

References

Agashe C et al (2009); Solar Energy Materials and Solar Cells 93, P 1256-1253

Bagheri Mohaghegi MM et al (2008); Physica B 403, P 2431-2437

Khan AF et al (2010); Applied Surface Science 256, P 2252-2258,

Kikuchi N et al (2002); Vacuum, 66 P 365-371

Moharrami F et al (2012); Solid films, 520, P 6503-6509

Maekava T et al (2001); Sensors and Actuators, B 80, P 51-58

Ouerfelli J et al (2008); Materials Chemistry and Physics, 112, P 198-201

Rani S et al (2007); Sensos and Actuators, B 122, P 204-210

Yin LT et al (2000); Sensors and Actuators, B 71, P 106-111