Thickness and oxygen partial pressure dependence on optical band gap of indium oxide by reactive evaporation method

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Abstract. Indium oxide film is deposited by reactive evaporation of indium in the presence of oxygen gas onto an unheated glass substrate. It was found that thickness of the film and partial oxygen pressure during the deposition affects the optical properties of the indium oxide thin film. We studied the optical band gap for different thickness and partial pressure keeping a constant annealing temperature. It was found that the band gap varies from 3.5 to 3.8 eV, as thickness of the film increased. The band gap energy had also shows the similar trend and it was also studied as a function of annealing temperature. A systematic investigation of the optical band gap as a function of thickness and oxygen partial pressure at different annealing temperature was carried out.

1. Introduction
Indium oxide (In$_2$O$_3$) is a wide band gap n-type oxide semiconductor. It has a low resistivity, which is an unusual property for a wide band gap material, compared with conventional semiconductors doped with impurities. The good conductivity of this film is a result of very high doping due to incomplete oxidation. Indium Oxide thin films are characterized by high transparency in the visible region of the spectrum and high reflectance in the infrared region.

Transparent conductive oxide (TCO) material is an interesting semiconductor owing to its unique properties of both high electrical conductivity and high optical transparency [1-2]. As a matrix for the generation of transparent conducting oxides, indium oxide (In$_2$O$_3$) has been the subject of numerous studies for liquid crystal displays [3], solar cell [4], sensors [5], nanowire technology [6], light emitting diodes, and other optoelectronic devices. In the present study, we have investigated the optical properties of InO thin film by reactive evaporation method on a glass substrate.

2. Experimental
The films of Indium Oxide (In$_2$O$_3$) were prepared by reactive evaporation technique using HINDHIVAC-12A4D high vacuum coating unit. Resistively heated Molybdenum (Mo) source in the form of boat was used for evaporation of Indium (purity 99.999%). The evaporation was carried out in the presence of oxygen plasma. The vacuum chamber was initially evacuated to base pressure $10^{-3}$ Pa using diffusion pump. Oxygen was then admitted to the chamber. By adjusting the valve the chamber pressure could be varied between 0.01 and 0.1 Pa during deposition. Optically flat glass slides were used as substrates. The cleaning procedure adopted was as follows: the films were kept in freshly prepared hydrochloric acid overnight and then washed with distilled water. The glass plates were then kept in a detergent solution and cleaned using isopropyl. Finally, the glass plates were cleaned with...
acetone. The thickness of these films was obtained by quartz crystal monitor. The thickness varied between 500Å -1200Å keeping deposition rate 0.5Å/s.

The films were placed on Muffle furnace and heated for different temperature in open air to investigate annealing effect. The films thus prepared were characterized optically. A UV-VIS double beam spectrophotometer was used to obtain the transmission spectrum of these films.

3. Results and discussion

Figure 1 shows a typical transmission curve of an In$_2$O$_3$ thin film with a thickness of 743Å. As can be seen from this figure, the transmission is high in the visible region. However, it depends on the partial pressure of oxygen during deposition [7] and thickness of the film [8].

From the transmission data, the absorption coefficient as a function of photon energy was calculated and plotted for the direct allowed transition by using the Tauc equation [9],

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

Where $E_g$ is the transition energy gap and $h\nu$ is the photon energy. Figure 2 shows the $(\alpha h\nu)^2$ vs $h\nu$ plots for various thicknesses. Extrapolation of linear region of such a curve gives the value of the band gap. The refractive index $n$ of the film was calculated using the formula [10]. Figure 3 shows the variation of refractive index with wavelength

$$n_f = \left[\frac{n_s(2 - T_{min}) + 2n_s(1 - T_{min})^{1/2}}{T_{min}}\right]^{1/2}$$

3.1 Influence of thickness on optical properties

The influence of the film thickness on the optical band gap was studied for films deposited 500Å to 1200Å thicknesses, with annealing temperature variation 200°C - 400°C. Figure 4 shows the variation of band gap energy as a function of thickness. The calculated band gap energy as a function of thickness, with different annealing temperature are listed in table 1. The results showed that the optical band gap was increased from 3.58-3.74eV by increasing the film thickness and it decreases with increase in annealing temperature. These results are consistent with other published results such as results of M.D Benoy et al [11] who attribute the increase in the band gap as a function of thickness was due to grain size growth and composition changes taking place in the sample.
3.2 Influence of oxygen partial pressure

Figure 5 shows the plot of \((\alpha h\nu)^2\) vs \(h\nu\) for indium oxide film of thickness 743Å deposited at different oxygen partial pressures and at different annealing temperature. Extrapolation of the linear region of the graph gives the band gap. The values are given in table 2. These values are somewhat higher than the bulk value about 3.5eV [12]. This shift is believed to be due to the Burstein effect, observed in the case of many conducting transparent oxides [13-14]. The band gap is found to increase with oxygen partial pressure. When the oxygen partial pressure is increased, transformation of InO to In\(_2\)O\(_3\) is accelerated.

**Table 1.** Optical band gap dependence on thickness and annealing temperature.

| Temp  | 500Å  | 700Å  | 743Å  | 900Å  | 1200Å |
|-------|-------|-------|-------|-------|-------|
| 200ºC | 3.66  | 3.68  | 3.71  | 3.74  |       |
| 300ºC | 3.62  | 3.63  | 3.65  | 3.69  | 3.71  |
| 400ºC | 3.58  | 3.60  | 3.62  | 3.63  | 3.65  |

**Table 2.** Optical band gap dependence on oxygen partial pressure and annealing temperature.

| Temp  | 3E-5mbar | 5E-5mbar | 7E-5mbar | 9E-5mbar | 19E-5mbar |
|-------|----------|----------|----------|----------|-----------|
| 300ºC | 3.59     | 3.61     | 3.63     | 3.65     | 3.71      |
| 360ºC | 3.58     | 3.60     | 3.62     | 3.64     | 3.69      |
| 400ºC | 3.56     | 3.58     | 3.60     | 3.62     | 3.66      |
4. Conclusion
Indium oxide thin film was deposited by reactive evaporation of indium in oxygen. We found that the thickness, annealing temperature and oxygen partial pressure dependence on the optical band gap of indium oxide film. We also had shown that the transmittance of annealed film was above 95% in visible region.

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