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XRD, UV-Vis-NIR and FT-IR Studies of ITO and Cr: ITO Thin Films Prepared by Electron Beam Evaporation Technique

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ABSTRACT. The Indium-tin-oxide (ITO) and Cr doped ITO thin films were prepared using electron beam evaporation technique. The prepared thin films were subjected to structural and optical properties. From the XRD it was observed that the films were crystalline in nature with cubic structure. The crystallite size was calculated using Scherer's relation and found that it was about 25 nm. The optical transmittance and absorbance spectra were recorded using UV-Vis-NIR spectrophotometer. From these, the optical band gap of ITO and Cr:ITO thin films were found to be 4.0 eV and 3.97 eV, respectively. The Fourier transform-Infrared spectroscopy study showed the peaks at 292, 519, 804, 957, 114, 1387 and 2985 cm^{-1} which are characteristic of In-O bonds.

Introduction. It is known that extensive work is being carried out on optical and electrical properties of wide band gap oxide semiconductors such as ZnO, TiO₂, SnO₂, In₂O₃, Cu₂O etc. [1-7]. Among the other oxide semiconductors, In₂O₃ is the one of the best suited materials for many electronic applications. It is a transparent, degenerate n-type wide band gap semiconductor with cubic structure in which the optical and electrical properties can be varied by doping of tin (Sn) or creating off stoichiometry. In In₂O₃ lattice if 10% of Tin (Sn) is doped the resultant material indium-tin-oxide is called as ITO [8, 9]. Due to its peculiar properties of high electrical conductivity and high optical transmittance in visible region it finds numerous applications such as nano electronics, opto electronics, sensor devices, flat panel displays and energy storage devices [10-18]. However, the studies of magnetic properties of ITO and impurity doped ITO thin films are meager. Recently continuous efforts are being put on magnetic properties of ITO and doped ITO nanoparticles, thin films and nanostructures. At present, this paper has been focused more on the structural and optical properties of ITO and Cr:ITO thin films and magnetic studies will be carried out in the future.

Experimental Details. The ITO and Cr doped ITO source materials were prepared using solid state reaction and studied their physical properties [12]. The same powder samples were taken here as source materials to prepare the ITO and Cr: ITO thin films on glass substrate. The films were prepared using electron beam evaporation technique [12A4D]. A base pressure of 5×10^{-6} mbar was created before coating the films. The total set up was kept in coating unit and the substrate temperature was raised to 350 °C and maintained the same temperature till the end of the coating.

The thicknesses of the films were found to be about 250 nm. X-ray diffractometer (D8 Advance, BRUKER) was used to establish structural aspects. The diffused reflectance spectra were recorded on UV-Vis-NIR Spectrophotometer (JASCO V-670). Fourier Transform Infrared (FT-IR) Spectroscopic analysis was carried using FT-IR Spectrophotometer (SHIMADZU).

Results and Discussion.

Structural Analysis. Figure 1 shows the XRD profiles of ITO and Cr doped ITO thin films. The Cr doped ITO thin films exhibited two more diffraction peaks in addition to pure ITO thin films. The diffraction peaks such as (2 2 1), (2 2 2), (3 2 1), (4 4 0), (4 0 0) and (6 2 2) were observed for Cr: ITO thin films which are characteristic of cubic structure of indium oxide [JCPDS 06-0416]. No other diffraction peaks other than indium oxide were observed in the XRD patterns. No significant change in the diffraction peak toward higher or lower diffraction angles. The crystallite size was calculated using Scherer's relation and found to be 25 nm. A slight decrease in lattice parameter was observed by adding Cr into the ITO lattice.

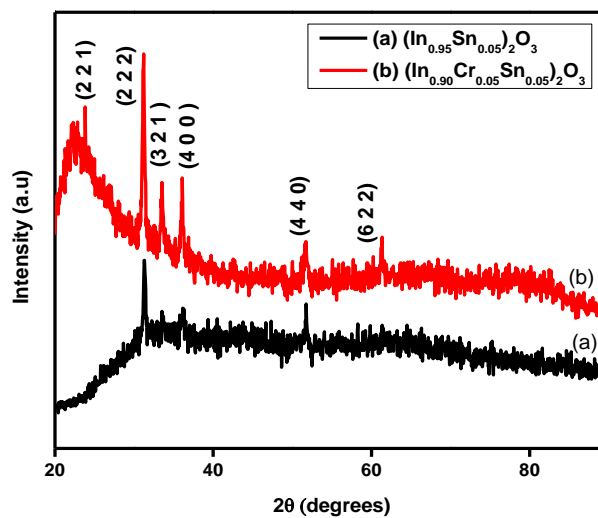


Fig. 1. XRD profile of ITO and Cr:ITO thin films.

Optical Properties. Figure 2 shows the optical transmittance spectra of ITO and Cr: ITO thin films prepared on glass substrates. From the figure it can be seen that the ITO thin films exhibited good optical transmittance about 70% in the visible region. The transmittance of the films decreased to large extent by doping chromium into the ITO lattice.

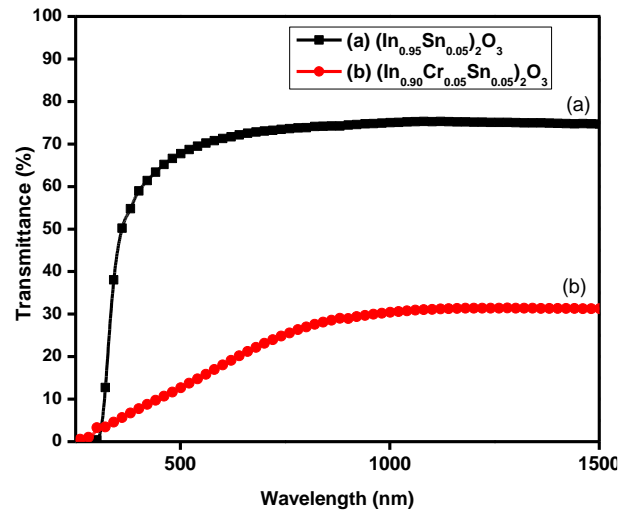


Fig. 2. Optical transmittance spectra for ITO and Cr:ITO thin films.

The optical band gap (E_g) of the films was determined from the optical transmittance data using Tauc's relation [19].

$$\alpha h\nu = (E_g - h\nu)^n \quad (1)$$

where n – depends on the kind of optical transition that prevails.

Here $n = 1/2$, as In_2O_3 is directly allowed n-type degenerate semiconductor. The optical band gap is obtained by plotting $(\alpha h\nu)^2$ versus the photon energy ($h\nu$) and by extrapolating of the linear region of the plots to zero absorption ($\alpha = 0$). The optical band gap E_g is obtained by plotting $(\alpha h\nu)^2$ versus the photon energy ($h\nu$) and by extrapolating the linear region of the plots to zero absorption ($\alpha = 0$). Fig. 3 shows the optical band gaps of ITO and Cr: ITO thin films. The pure ITO thin films exhibited a band gap of 4.0 eV and Cr: ITO thin films exhibited a band gap of 3.95 eV. The observed band gap is almost equal to that of band gap of bulk ITO [20].

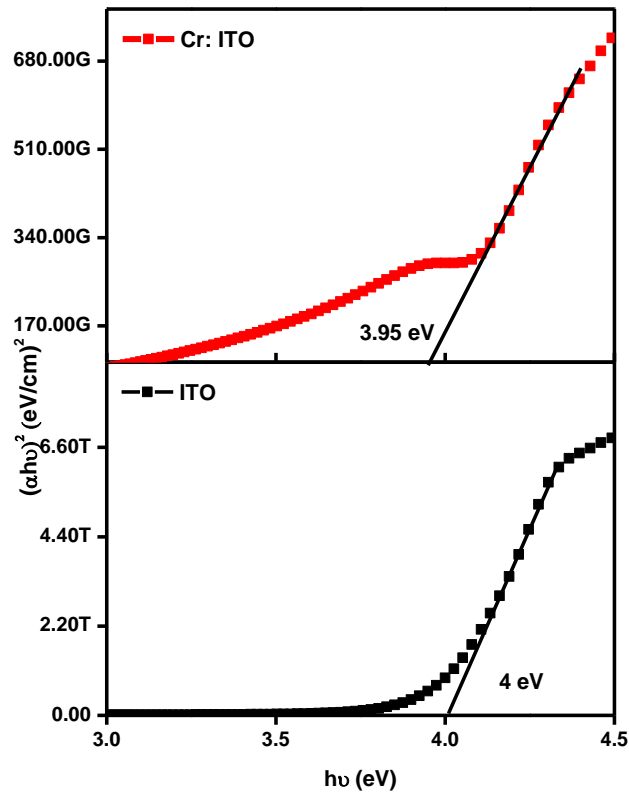


Fig. 3. Optical band gaps of ITO and Cr:ITO thin films.

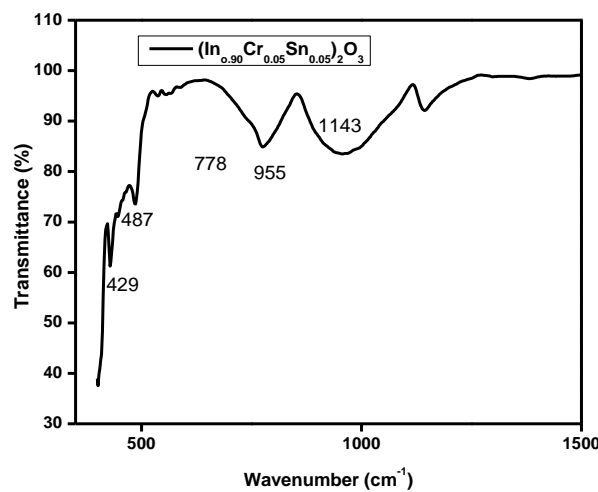


Fig. 4. FT-IR spectra of Cr: ITO thin films.

Fig. 4 shows the FTIR spectra of Cr: ITO thin films recorded at room temperature. The same trend was observed in pure ITO thin film. In_2O_3 exhibits intense bands around 419 and 440 cm^{-1} attributed to In-O lattice stretching vibrations [21].

Summary. ITO and Cr: ITO thin films were prepared using electron beam evaporation technique and studied for their structural and optical properties. Both ITO and Cr: ITO thin films were in cubic structure with crystallite size of 24 nm. No new diffraction peaks related to nickel was found in XRD. A band gap of 4.0 eV was observed for ITO thin films and it decreased to 3.95 eV by doping Cr into the ITO lattice. The FT-IR studies revealed the characteristics of In_2O_3 lattice.

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