Microstructure and dielectric function modelling by spectroscopic ellipsometry and energy electron loss spectroscopy of In_2O_3:Sn thin films

Conference or Workshop Item

Microstructure and dielectric function modelling by Spectroscopic Ellipsometry and Energy Electron Loss Spectroscopy of In_2O_3:Sn thin films

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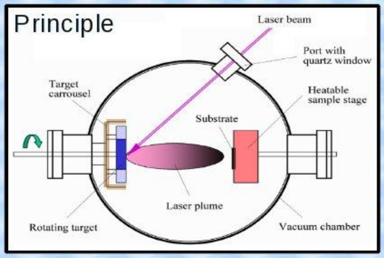
Introduction

Indium tin oxide (ITO) is a semiconducting material combining high conductivity and high transparency in the visible range. It is the most widely used transparent conducting oxide in applications such as flat panel displays. In this work, ITO thin films were deposited by Pulsed Laser Deposition (PLD) onto transparent substrates (Corning 1737 glass). Deposition conditions (substrate temperature (T_s) and oxygen pressure ($P(O_2)$)) were changed to generate a variety of microstructures and electro-optical properties. Similar film thicknesses were used to avoid any change of carrier concentration (N). The dielectric function/complex refractive index were derived from spectroscopic ellipsometry using the Cauchy model in the 1.5-5.5 eV range and from Electron Energy Loss Spectroscopy for samples grown at RT, 200 and 400°C. Kramers-Kronig analysis of the single-scattering distribution (SSD) enabled the extraction of the real and imaginary parts of the dielectric function/complex refractive index.

Pulsed Laser Deposition (PLD)

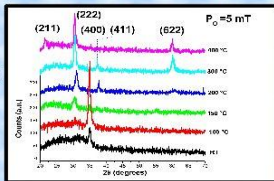
Principle

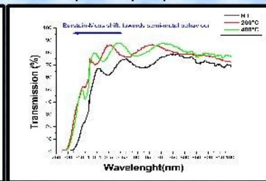


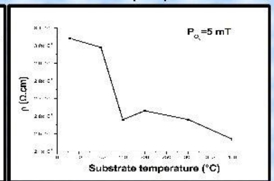
Substrate temperature (T_s) and Oxygen pressure $P(O_2)$ varied

Structural characterisation | Optical properties | Electrical properties

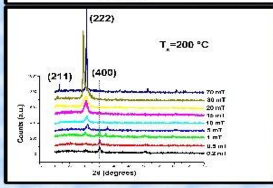
T_s - varied

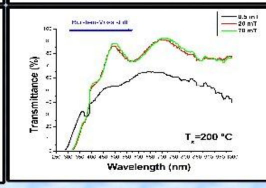


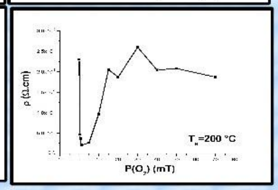




$P(O_2)$ - varied





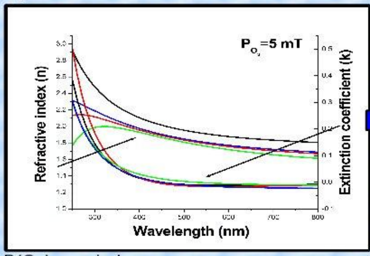


Ellipsometry: 1.5-5.5 eV range

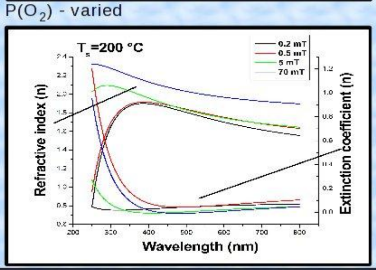
Use of Cauchy model:

$$n(\lambda) = A + \frac{B\cdot 10^4}{\lambda^2} + \frac{C\cdot 10^9}{\lambda^4}, \quad k(\lambda) = D\cdot 10^{-5} + \frac{E\cdot 10^4}{\lambda^2} + \frac{F\cdot 10^9}{\lambda^4}$$

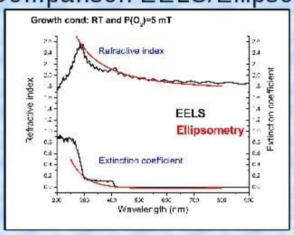
T_s - varied

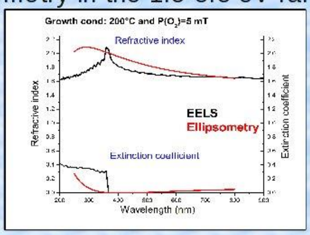


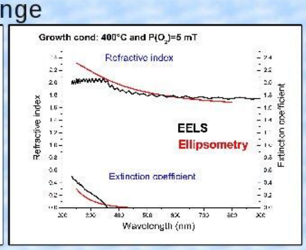
$P(O_2)$ - varied



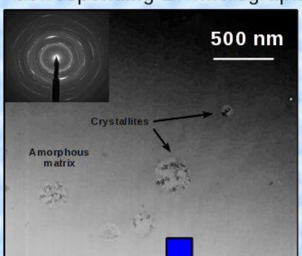
Comparison EELS/Ellipsometry in the 1.5-5.5 eV range

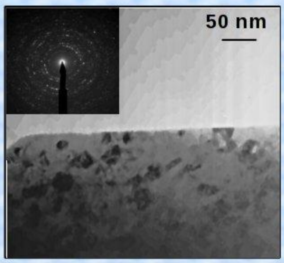


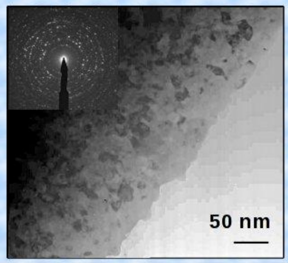




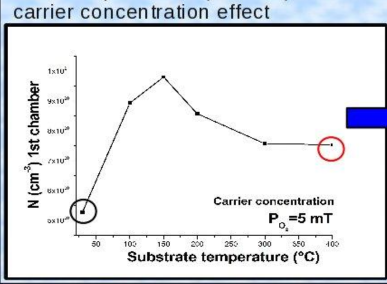
Corresponding BF micrographs:

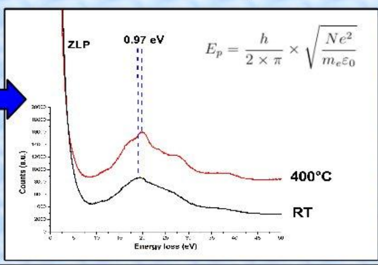






Plasmon peak shift (0.97 eV) between RT and 400°C: carrier concentration effect





$$E_p = \frac{h}{2\times\pi}\times\sqrt{\frac{Ne^2}{m_e\varepsilon_0}}$$

EELS parameters spectra processing (EL/P 3.0 - Gatan):

(1) Raw spectrum. FWHM=0.9-1.4 eV - t=0.4/0.6*IMFP - β=5 mrads E_0=200 kV
(2) Deconvolution with a hole spectrum
(3) Removing of multiple scattering: Fourier-log deconvolution
(4) Single scattering distribution (SSD) obtained
(5) SSD fed into KRAKRO (fortran program – R.F. Egerton)
(6) Normalisation via a known optical refractive index taken from ellipsometry results (800 nm)

Agreement between Hall-effect, EELS measurements and optical data ("Burstein-Moss shift"=widening of the band gap=blocking of the lowest states in the conduction band above the critical Mott density))

Conclusion:

In the low energy range, the EELS results showed a reasonable agreement with the ellipsometry except at 200°C. This could be due the higher thickness of the specimen. Moreover, normalisation of the energy-loss function was accomplished using the refractive index. Normalisation will also have to be performed with an inelastic mean free path and the results compared with the present data. Increasing T_s and $P(O_2)$ resulted in more (222)-orientated structures, respectively lower/higher refractive indices (n) and lower extinction coefficients (k). Extinction coefficients were found to be very sensitive to the crystallinity and stoichiometry.