**Supporting Information**

“**Evaluation of** **spray pyrolysed In: ZnO nanostructures for CO gas sensing at low concentration**”

Aninamol Ani1, Poornesh P1\*, K K Nagaraja1,2, E. Kolesnikov2, Igor V. Shchetinin2, Albin Antony1, Suresh D Kulkarni3

1Department of Physics, Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal, Karnataka, 576104, INDIA

2National University of Science and Technology “MISiS“, Leninskiy Pr. 4, Moscow, 119049, Russian Federation

3Department of Atomic and Molecular Physics, Manipal Academy of Higher Education, Manipal, Karnataka, 576104, INDIA

\* Corresponding author: Poornesh P ([poorneshp@gmail.com](mailto:poorneshp@gmail.com), [poornesh.p@manipal.edu](mailto:poornesh.p@manipal.edu))

*S1. Optical Properties*

The UV-VIS spectroscopic analysis was performed to extract the values of transmittance, bandgap and Urbach energy of the films. The undoped and IZO films are highly transparent and showed excellent optical transmittance of 80% to 95% as evident from Fig. S1.1. The transmittance oscillations in the range 450-1100 nm suggests the films have smooth interfaces which further supports our observation on low RMS roughness of the films.

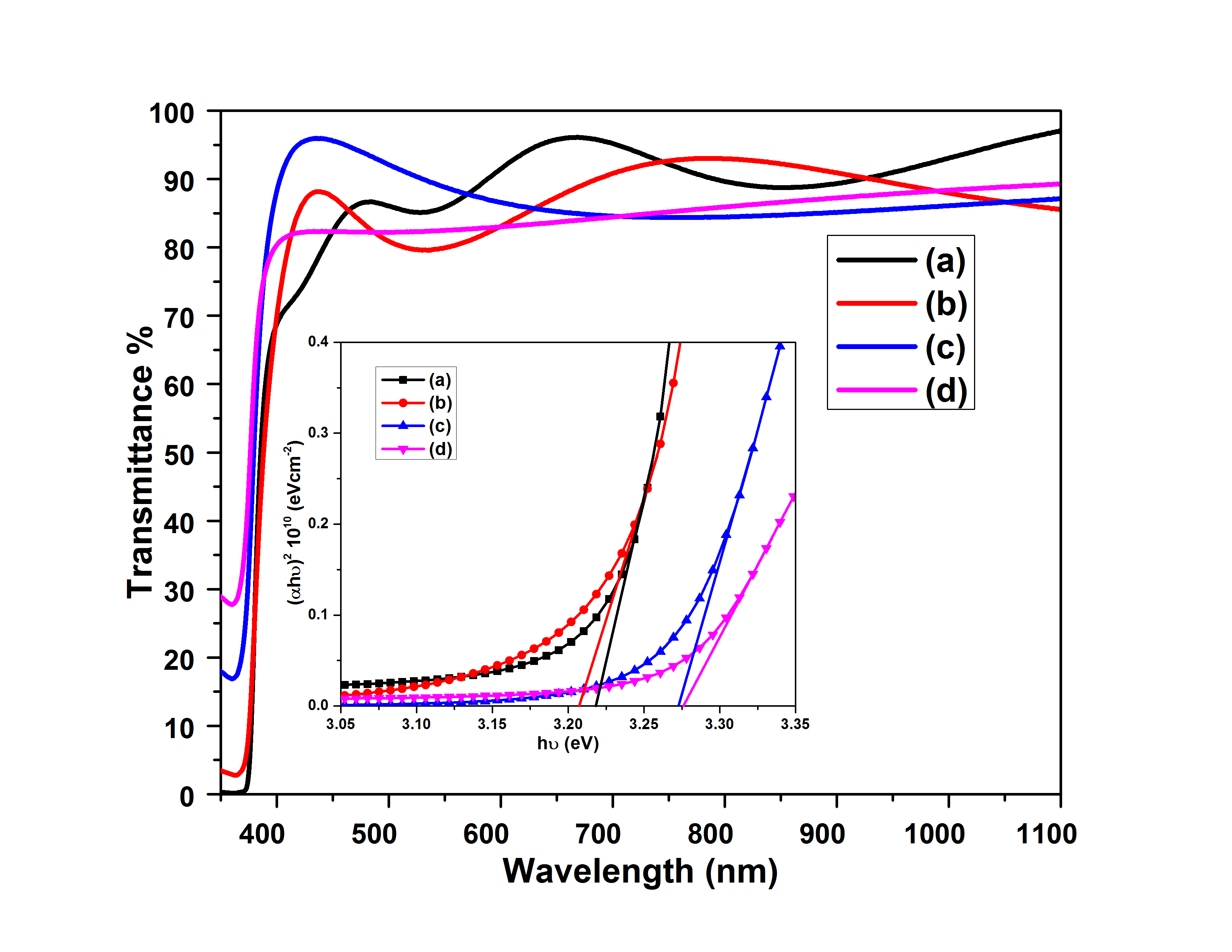


Fig. S1.1: Transmittance spectra of (a) undoped (b) 5 wt% (c) 10 wt% and (d) 15 wt% IZO thin films.

(Inset: Tauc Plot)

The absorption coefficient ( ) was found using the Beer-Lamberts law [42] given by,

(1)

Where t is the thickness of the films obtained and T is the transmittance achieved by the films. The bandgap of the films are obtained from Tauc plot which is a function of 2 versus employing Tauc’s relation [1],

)*m*  (2)

where hdescribes the photon energy, A is the energy-independent constant different for different transitions and whose value lies between 107 and 108 m-1, Eg represents the bandgap energy and m is a constant which decides the type of transitions and is assumed as ½ for direct transitions and 2 for indirect transitions [1]. The inset of figure 5 depicts the Tauc plot of undoped and IZO films. In our case, we have taken it as ½, as ZnO proves as a direct bandgap semiconductor. The bandgap of the undoped and IZO films are well within the range of standard ZnO thin films. To study the spread of disorders in the films, Urbach energy was obtained from the Urbach empirical rule represented by the exponential equation [1],

(3)

Where is considered as a constant and EU represents the Urbach energy of the localized states in bandgap. The graph of ln versus gives the Urbach tail. The linear portion in the bandgap energy region is plotted and it is linearly fitted to find the slope. The reciprocal of the slope gives the Urbach energy from the straight-line equation. The Urbach energy plot is shown in Fig. S1.2. The energy gap and Urbach energy values are given in Table S1.

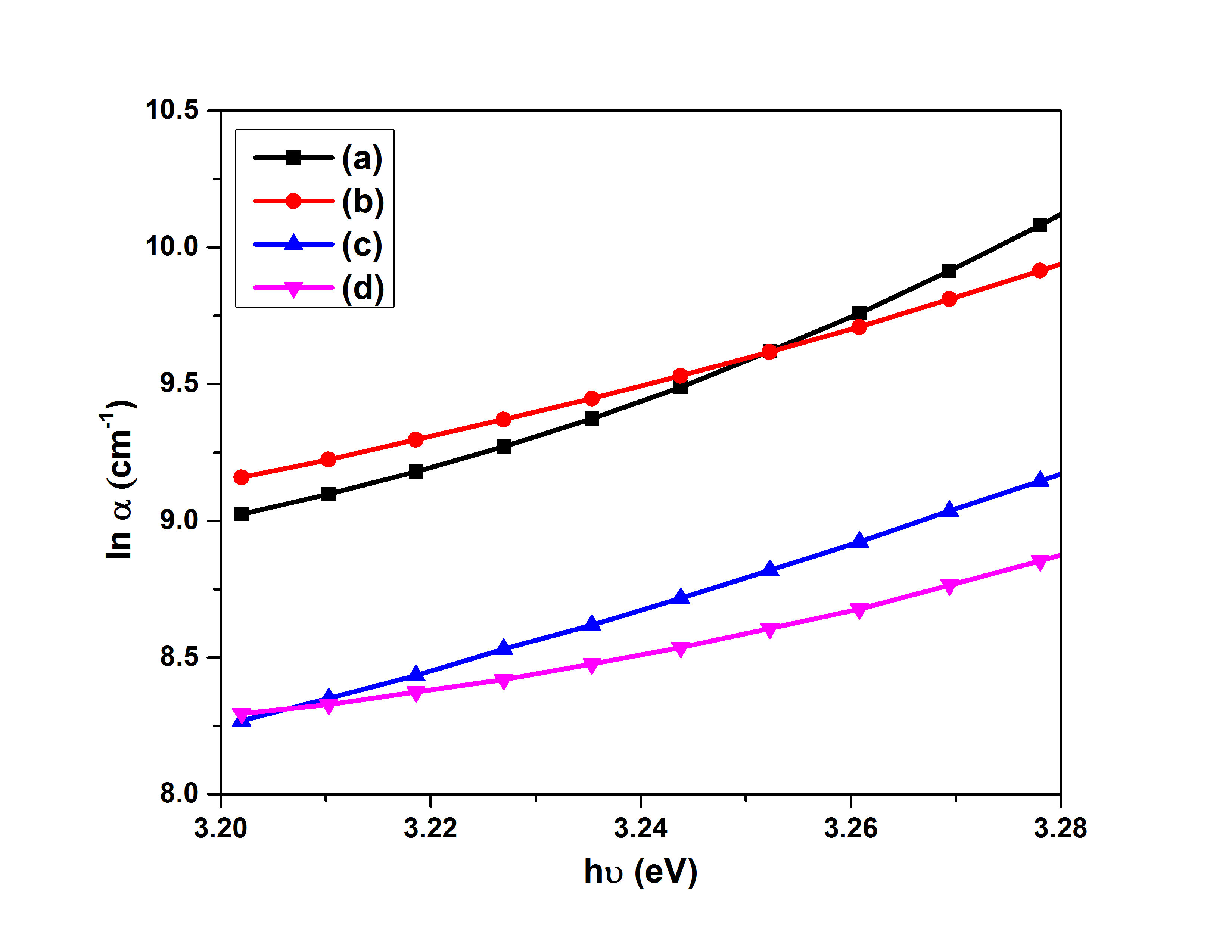


Fig.S1.2: ln v/s plot of (a) undoped (b) 5 wt% (c) 10 wt% and (d) 15 wt% IZO thin films.

Table S1: Band gap and Urbach energy of undoped and IZO thin films.

|  |  |  |
| --- | --- | --- |
| Doping concentration  (wt% In) | Band gap energy, Eg  (eV) | Urbach energy, EU  (eV) |
| undoped | 3.218 | 0.069 |
| 5 | 3.207 | 0.098 |
| 10 | 3.272 | 0.085 |
| 15 | 3.276 | 0.129 |

*S2. XRD comparison of indium oxide with 15 wt% In: ZnO*

The ZnO crystallises in hexagonal wurtzite structure whereas indium oxide (In2O3) has cubic structure. The most prominent planes in ZnO are (002) and (101) at around 34.3 and 36.15 respectively whereas In2O3 has (222) and (440) as the prominent planes in most cases at 30.8 and 50.3 respectively. The obtained 15 wt% In:ZnO has the standard peaks of ZnO which confirms the structural stability after doping with indium [2, 3]. Table S2 shows the comparison of diffraction peaks of In2O3 and 15 wt% In:ZnO.

Table S2: Comparison of diffraction peaks of In2O3 and 15 wt% In:ZnO

|  |  |  |
| --- | --- | --- |
|  | 2θ (deg.) | (hkl) |
| **In2O3**  **(ICSD-01-088-2160)**  **[3]** | 21.40 | (211) |
| 30.80 | (222) |
| 34.80 | (400) |
| 38.40 | (411) |
| 41.30 | (332) |
| 44.50 | (431) |
| 50.30 | (440) |
| 55.60 | (611) |
| 65.90 | (444) |
| 70.0 | (633) |
| 74.60 | (800) |
| 79.20 | (653) |
| **15 wt% In:ZnO**  **[2]** | 31.73 | (100) |
| 34.31 | (002) |
| 36.15 | (101) |
| 47.52 | (102) |
| 56.55 | (110) |
| 62.81 | (103) |
| 68.0 | (112) |

**References**

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