Supplementary information

Variation of electrical properties in thickening Al-doped ZnO films: Role of defect chemistry

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Determination of the crystallite size

Average crystallite size can be estimated from the measured full width half maximum (FWHM) of the (002) peak in the XRD pattern using the below Scherer equation:[1]

$$d = \frac{0.9 \cdot \lambda}{B \cos\theta} \qquad (1)$$

Here, B is denoted as FWHM, θ is the Bragg diffraction angle, d is the average crystallite size and λ is the wavelength of the incident X-ray radiation.

XPS data interpretation

All the measured X-ray Photoelectron Spectroscopy (XPS) O 1s spectra were referenced with respect to impurity C 1s line (284.6 eV) binding energy. The asymmetric O 1s spectra were deconvoluted into three components centred at 530.4 ± 0.1 eV, 531.4 ± 0.1 eV and 532.2 ± 0.1 eV respectively. The highest binding energy constituent (denoted as O_C) positioned at 532.2 eV suggested the presence of the loosely bound oxygen on the surface of the AZO films,e.g $-CO_2$ group, adsorbed O_2 and H_2O groups, whereas, lowest binding energy component located at 530.4 eV (denoted as O_A) suggested the presence of the O_2^-ions in ZnO wurtzite structure.[2,3] The occurrence of the medium binding energy component centred at 531.4 eV (denoted as O_B) could be due to the presence of the O_2^- ions in Al_2O_3.[4] The

intensity ratio of O_A to O_C is an important parameter which quantifies the presence of chemisorbed oxygen on the surface of AZO films. The intensity ratios of O_A to O_C for the AZO films deposited for 15, 60 and 120 mins are calculated to be 0.46, 0.85 and 0.79 respectively. Similarly, the intensity ratios of O_B to O_C quantifies the formation of Al_2O_3 for these films. They are 0.053, 0.122 and 0.200 for the above durations respectively.

Table S1. Spectral positions of deconvoluted peaks as determined by employing Photoluminescence (PL) spectroscopy on the Al-doped ZnO films deposited on soda lime glass substrates by RF magnetron sputtering at *t* varying in the range of 15 to 120 mins.

Deposition time	UV	Violet	Blue	Green	Yellow	Orange	Red
(mins)	100 - 380 (nm)	380-449 (nm)	450- 497 (nm)	498- 569 (nm)	570 - 589 (nm)	590 - 619 (nm)	620 - 750 (nm)
15	376.06	419.09	-	521.55	-	602.597	723.24
30	376.23	417.71	-	517.53	-	601.32	708.23
45	376.25	417.25	-	503.246	570.12	-	702.57
60	376.28	426.49	465.19	-	-	-	-
75	376.06	427.92	468.05	509.61	-	-	-
90	376.14	427.40	480.09	549.74	-	-	-
105	376.06	417.27	495.88	533.50	-	-	675.84
120	377.92	418.92	491.37	532.07	-	-	644.15

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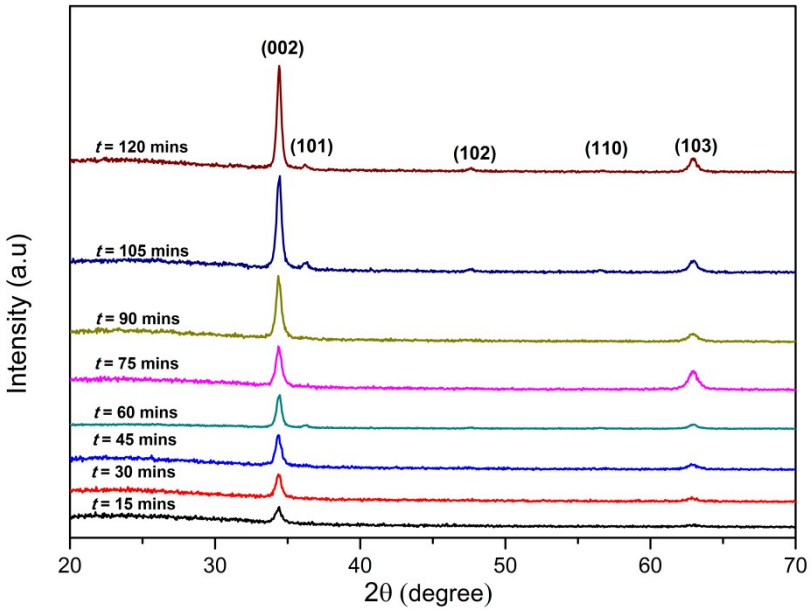

Fig. S1. X-ray diffraction pattern of Al-doped ZnO films deposited on soda lime glass substrates by RF magnetron sputtering at *t* varying in the range of 15 to 120 mins.

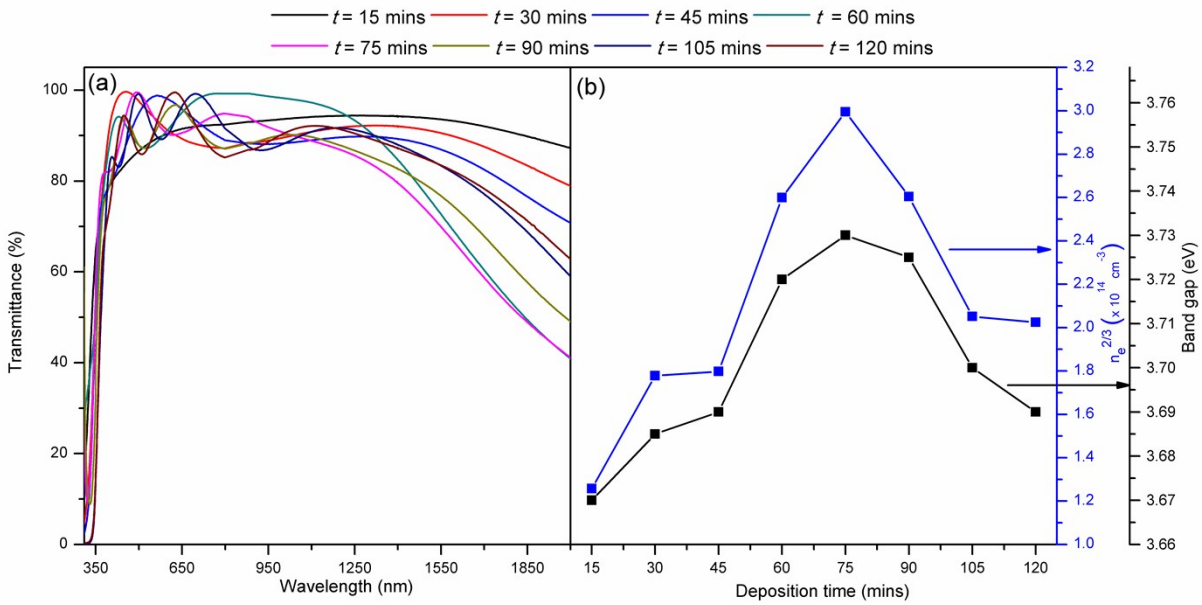

Fig. S2. (a) Optical transmission spectra (b) variation in optical band gap (E_g) and plot of $n_e^{2/3}$ of Al-doped ZnO films deposited on soda lime glass substrates by RF magnetron sputtering at *t* varying in the range of 15 to 120 mins.

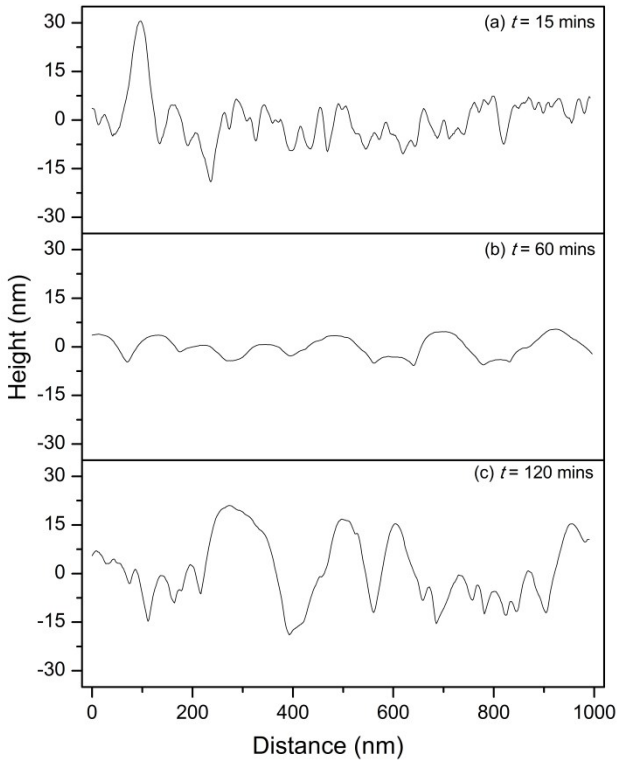

Fig. S3. AFM topography line section analysis of height (a - c) of the Al-doped ZnO films deposited on soda lime glass substrates by RF magnetron sputtering at *t* varying in the range of 15 to 120 mins.

References

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