

Supporting Information

Room-temperature tilted-target sputtering of highly transparent and low sheet resistance Al doped ZnO electrodes

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S.1 Electrode structural (XRD) and morphological (AFM, SEM) characterization

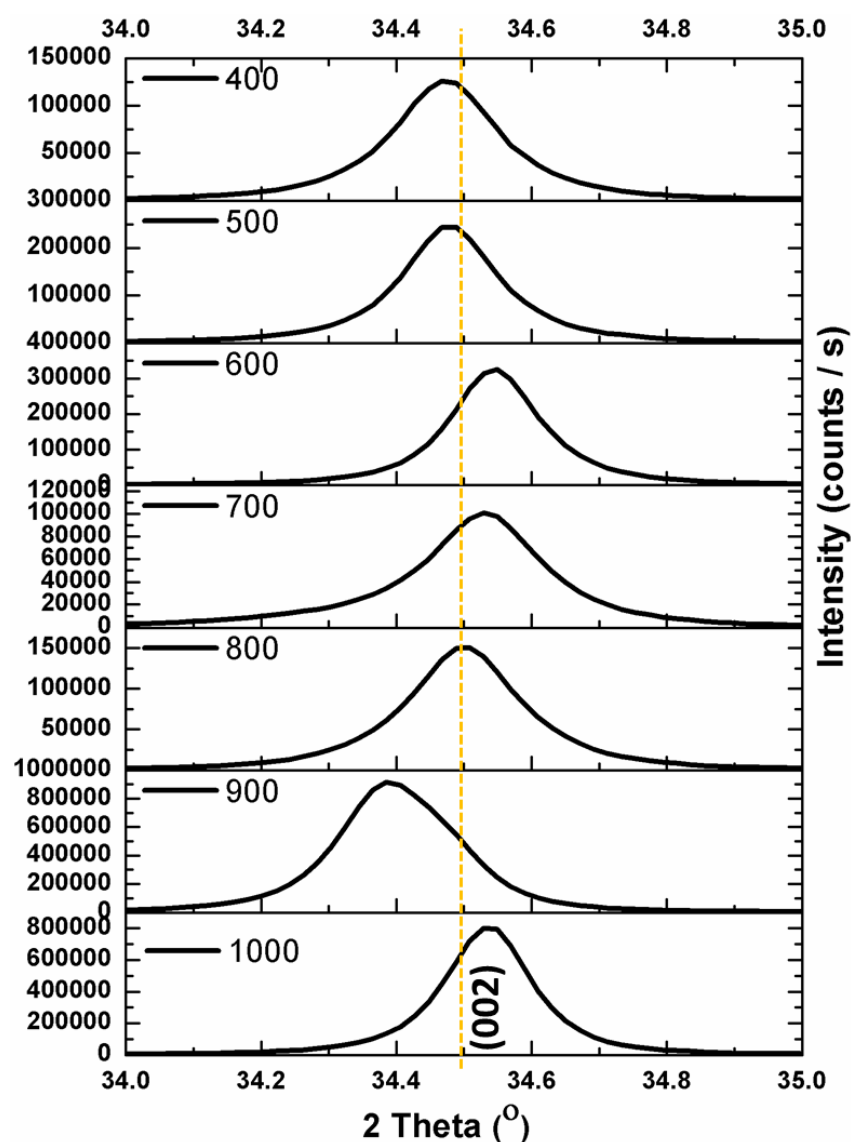


Figure S1. XRD patterns of AZO films of different thicknesses ranging from 400 nm to 1000 nm prepared on glass substrates. The (002) diffraction line is noted at 34.5°, which is reported for bulk ZnO powder.

Table S1: structural properties and calculated parameters as a function of AZO film thickness from the XRD characterization study.

Sample details	2 θ (°)	d (Å)	FWHM (°)	Area of (002) XRD peak	C (Å)	Average crystallite size (Å)	σ [GPa]
400 nm	34.473	2.599	0.169	34428	5.199	492	+0.31
500 nm	34.479	2.599	0.152	60672	5.198	545	+0.36
600 nm	34.545	2.594	0.141	74393	5.189	590	+0.76
700 nm	34.527	2.596	0.194	30946	5.192	429	+0.62
800 nm	34.500	2.597	0.176	42960	5.195	473	+0.50
900 nm	34.535(1)*	2.605	0.173	246178	5.209	481	+0.18
	34.374(2)*	2.607	0.137	-	5.214	604	-0.36
	34.461(2)*	2.600	0.120	-	5.200	692	+0.27
1000 nm	34.535	2.595	0.135	178413	5.190	614	+0.71

Where (1)* and (2)* indicate consideration of the (002) XRD diffraction line as a single Gaussian and deconvolution of two Gaussians, respectively for the stress/strain calculation for the 900 nm thick AZO film.

Equations used to calculate the structural parameters from the XRD:

Hexagonal wurtzite structure lattice constant relation:

$$\frac{1}{d^2} = \frac{4}{3} \left(\frac{h^2 + hk + k^2}{a^2} \right) + \frac{l^2}{c^2}$$

For the (002) plane of diffraction, lattice constant $C = 2 \times d$ (in angstrom units)

Average crystallite size calculated using the Scherrer formulae

$$\text{Average crystallite size} = \frac{0.9\lambda}{\beta \cos \theta}$$

Where λ is the Cu target $K_{\alpha 2}$ X-ray line wavelength 1.540562 Å, β is full width at half maximum (FWHM) of the XRD diffraction peak in radian units and θ is diffraction plane angle for the FWHM.

Stress in the film was calculated by the equation, $\sigma = -233 \left(\frac{c - c_0}{c_0} \right)$ G Pascal

where, C is the lattice constant of the film under study and C_0 is the lattice constant of the bulk ZnO powder (5.206 Å). The direction of the stress is in the film parallel to the surface of substrate. Positive (negative) sign of the stress value indicate tensile (compressive) stress in the film plane developed because of the strain induced in the direction of C-axis (normal to the plane of the film surface) for the oriented (002) films.

S.2 Optical constants for the OPV device stack layers used in this study (as measured from the spectroscopic ellipsometry).

Table S2. Thickness and surface roughness of the AZO films prepared at various target tilt angles extracted from the spectroscopic ellipsometry psi/delta data fittings.

Ellipsometry		
Target tilt	t [nm]	Roughness [nm]
16.2°	353	2.6
20.8°	362	3.7
23.8°	321	2.8
31.3°	322	6.5
38.8°	290	5.9

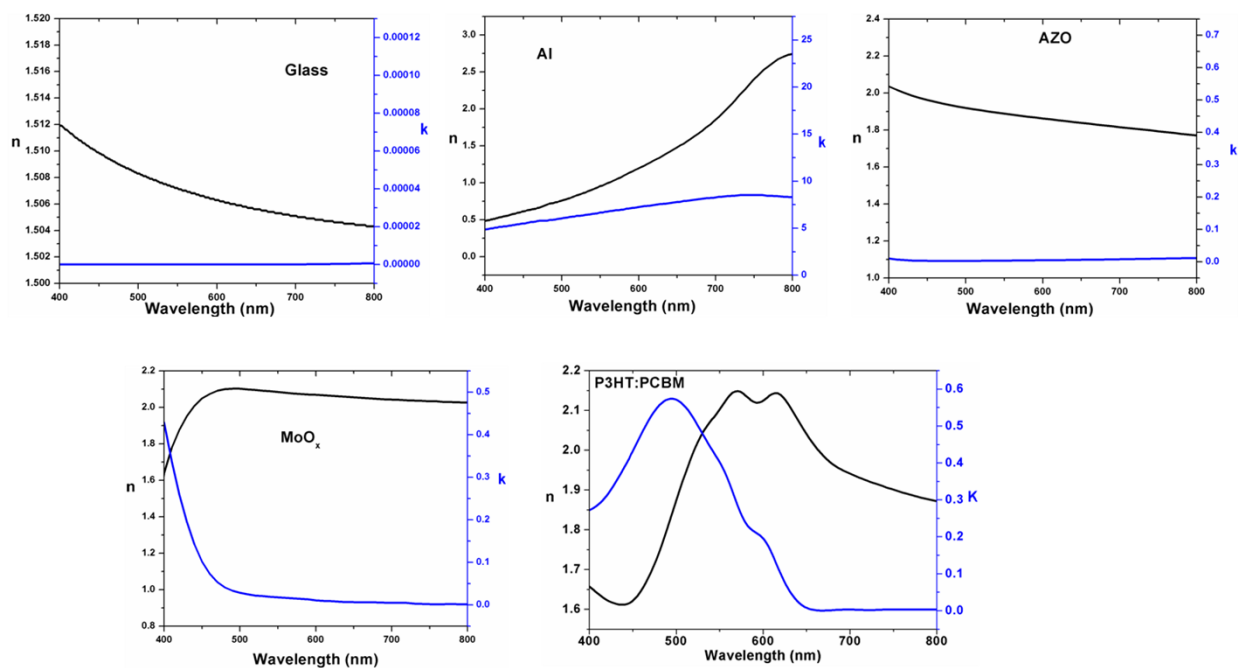


Figure S2. Optical constants refractive index (n) and extinction co-efficient (k) of the stack layers used for the OPV device optical modelling.