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Superior photoresponse MIS Schottky barrier diodes with nanoporous:Sn-WO_3 films for ultraviolet photodetector application

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Supporting Information

The significant structural parameters such as crystallite size (D) dislocation density (δ), micro-strain (ε), stacking fault (SF) and texture coefficient (TC) of the Sn-WO_3 films were calculated using the following equations.

$$D = \frac{0.89\,\lambda}{\beta \cos\theta} \tag{1}$$

$$\delta = \frac{1}{D^2} \tag{2}$$

$$\varepsilon = \frac{\lambda}{D\,sin\theta} - \frac{\beta}{tan\theta} \tag{3}$$

$$SF = \left[\frac{2\pi^2}{45(3\,tan\theta)^{\frac{1}{2}}}\right]\beta \tag{4}$$

Where D is the crystallite size, λ is the wavelength, β is the full width half the maximum (FWHM) of the diffraction peak and θ is the angle of diffraction.

The texture coefficient (TC) is the essentials parameter to analyze the diffraction peaks of the films, which is calculated from the following relation.

$$TC = \frac{I_0(h_ik_il_i)}{I_s\,(h_ik_il_i)}\left[\frac{1}{N}\sum\frac{I_0(h_ik_il_i)}{I_s\,(h_ik_il_i)}\right]^{-1} \tag{5}$$

Where TC is the texture coefficient, n is the reflection number, I_S is the standard intensity and I_o is the observed intensity.

Optical band gap values of the Sn-WO_3 composite films were calculated using the following formula.

$$(\alpha hv)^{1/2} = A\,(hv - E_g) \tag{6}$$

Where α is the absorption coefficient, h is the Planck's constant, A is the constant and E_g is the band gap energy.

The optical parameters of the Sn-WO_3 composite films were calculated using the following relations.

$$\alpha = \frac{\ln\left(\frac{1}{T}\right)}{t} \tag{7}$$

$$k = \frac{\alpha\lambda}{4\pi} \tag{8}$$

$$\sigma_{Opt} = \frac{nc\alpha}{4\pi} \tag{9}$$

$$n = \frac{1+R}{1-R} \pm \tag{10}$$

Where α is the absorption coefficient, n is the refractive index, T is the transmittance, t is the thickness of the film, c is the velocity of light and λ is the wavelength.

The electrical resistivity (ρ) of the coated films were calculated using the following equation and are listed in Table 4.

$$\rho = R\left(\frac{A}{t}\right)\Omega cm \tag{11}$$

Where ρ is the resistivity, R is the resistance, A is the area of the film and t is the film thickness.

The activation energy (E_a) of the films were deduced from the Arrhenius plots (Fig. 10) and using the following equation.

$$\sigma_{dc} = \sigma_0 \exp\left(\frac{-Ea}{k_B T}\right) \tag{12}$$

Where E_a activation energy, T is the temperature, σ_{dc} is the conductivity, σ_0 is the pre-exponential factor and k_B is the Boltzmann constant.

The current conduction mechanism of the Cu/p-Si Schottky diode through nanoporous:Sn-WO_3 layer was explained by thermionic emission theory (TET) using the following equations .

$$I = AA^* \, T^2 \, exp\left(-\frac{q\phi_B}{K_B T}\right)\left[exp\left(\frac{qV}{nK_B T} - 1\right)\right] \tag{13}$$

Here,

$$I_0 = AA^* \, T^2 \, exp\left(-\frac{q\phi_B}{K_B T}\right) \tag{14}$$

Where I_o is the reverse saturation current, q is the charge of an electron, V is the bias voltage, n is the ideality factor, Φ_B is the effective barrier height, A is the active area of the diode, K_B is the Boltzmann constant, T is the temperature and A* is the effective Richardson constant.

The ideality factor (n) of the diode was deduced from the intercepts of semi-logarithmic plots of ln J vs voltage and using the following equation.

$$n = \frac{q}{k_B T}\left(\frac{d(V)}{d(ln(I))}\right) \tag{15}$$

The effective barrier height of the Cu/Sn-WO_3/p-Si diode was calculated by the following expression.

$$\phi_B = \frac{K_B T}{q} In\left(\frac{AA^* \, T^2}{I_0}\right) \tag{16}$$

The photo-sensitivity (P_S), responsivity (R), external quantum efficiency (EQE) and specific detectivity (D*) of of the diodes were calculated by the following equations.

$$P_s\,(\%) = \frac{I_{Ph} - I_D}{I_D} \times 100 \tag{17}$$

$$R = \frac{I_{Ph}}{PA} \tag{18}$$

$$QE = \frac{Rhc}{q\lambda} \tag{19}$$

$$D^* = \frac{R}{(2qI_D)^{1/2}} \tag{20}$$

Where I_D is the dark current, I_{Ph} is the photocurrent, A is the area of the diode, h is the Planck's constant, p is the irradiation of the lamp, c is the light velocity, q is the charge of electron and λ is the wavelength.

Supplementary Figures

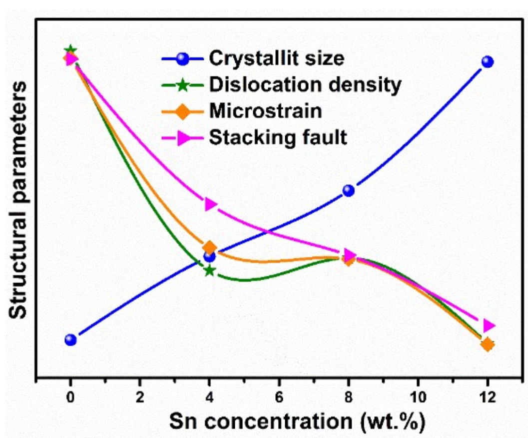

Fig. S1. Structural parameters vs Sn concentration (wt.%) for Sn-WO_3 films.

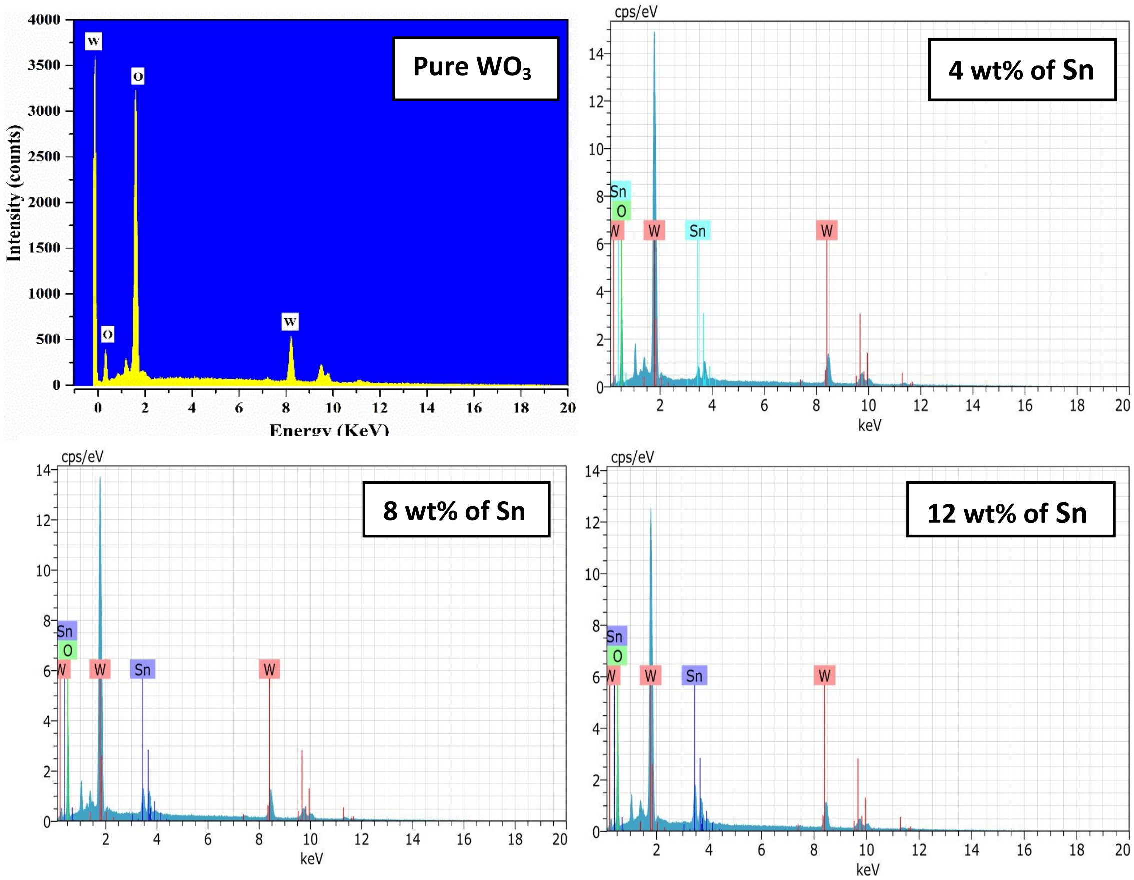

Fig. S2. EDX spectrum of Sn-WO_3 films with different concentrations of Sn.

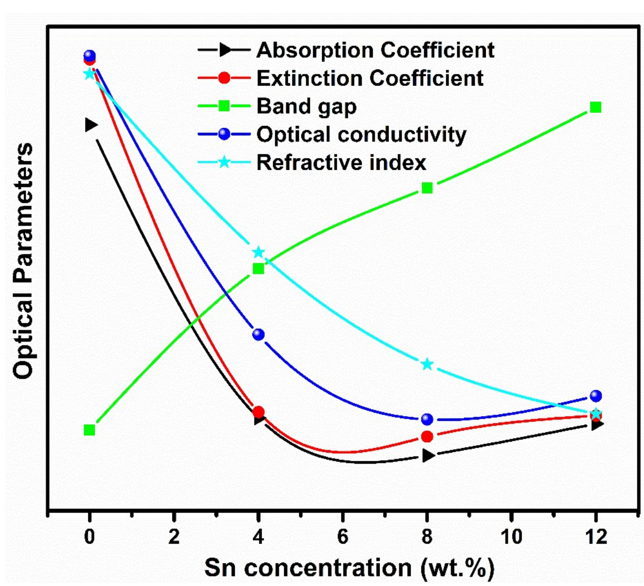

Fig. S3. Optical parameters vs various Sn concentrations (wt%) in WO_3 films.

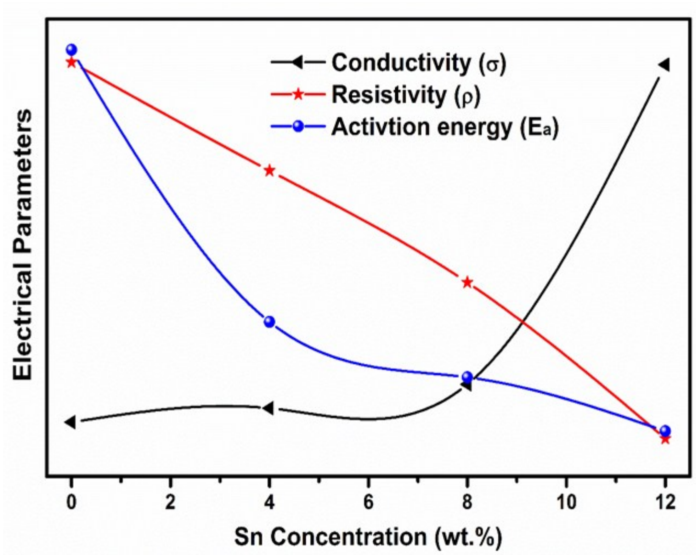

Fig. S4. Electrical parameters vs different Sn concentrations for Sn-WO_3 films.

Supplementary Tables

Table S1 Structural parameters of (002), (020) and (200) planes with different Sn concentration.

Sn Concentrations (wt.%)	Diffraction angle 2θ (°)	Inter planar distance (d) (Å)	FWHM (Radians)	Crystallite size (D) (nm)	Micro strain (ε)	Dislocation density (δ) (× 10^{14} lines m^{-2})	Stacking fault (SF) (× 10^{-2})	Texture coefficient (TC)
0	23.34	3.8106	0.00429	33.0	1.0511	9.1819	0.2142	0.914
	23.85	3.7304	0.00343	41.2	0.8401	5.8655	0.1735	0.973
	24.56	3.6242	0.00343	41.3	0.8390	5.8500	0.1764	1.172

4	23.22	3.8300	0.00257	54.9	0.63084	3.3069	0.1281	0.234
	23.72	3.7509	0.00343	41.2	0.84037	5.8684	0.1729	0.249
	24.43	3.6435	0.00343	41.3	0.83926	5.8529	0.1758	0.376
8	23.07	3.8547	0.00257	54.9	3.30872	0.6310	0.1277	0.432
	23.52	3.7820	0.00343	41.2	5.87265	0.8406	0.1721	0.348
	24.27	3.6667	0.00323	43.9	5.18635	0.7900	0.1649	0.832
12	23.29	3.81927	0.00257	54.9	3.30615	0.6307	0.1284	1.134
	23.98	3.71042	0.00343	41.3	5.86273	0.8399	0.1740	0.231

Table S2 Atomic percentage of Sn-WO_3 composite thin films.

Sn concentrations (wt. %)	**Atomic ratio (%)**		
	Sn	**W**	**O**
0	-	23.52	76.48
4	1.83	13.64	84.53
8	2.97	12.18	84.85
12	4.20	11.20	84.60