Supporting Information for New Journal of Chemistry

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), microstrain (ε), stacking fault (SF) and texture coefficient (TC) of the Sn-WO$_3$ films were calculated using the following equations.

\[ D = \frac{0.89 \lambda}{\beta \cos \theta} \]  
(1)

\[ \delta = \frac{1}{D^2} \]  
(2)

\[ \varepsilon = \frac{\lambda}{D \sin \theta} - \frac{\beta}{\tan \theta} \]  
(3)

\[ SF = \left[ \frac{2\pi^2}{45(3 \tan \theta)^2} \right]^{1/2} \beta \]  
(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.
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.

\[(ahv)^{1/2} = A (hv - E_g)\]

Where $\alpha$ 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.

\[\ln \left(\frac{1}{T}\right) = \frac{\alpha}{t}\]

\[k = \frac{\alpha \lambda}{4\pi}\]

\[\sigma_{opt} = \frac{nc\alpha}{4\pi}\]

\[n = \frac{1 + R}{1 - R} \pm\]

Where $\alpha$ 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 $\lambda$ is the wavelength.

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

\[\rho = R \left(\frac{A}{t}\right) \Omega cm\]

Where $\rho$ 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.
\[ \sigma_{dc} = \sigma_0 \exp \left( \frac{-E_a}{k_B T} \right) \]  

(12)

Where \( E_a \) is the activation energy, \( T \) is the temperature, \( \sigma_{dc} \) is the conductivity, \( \sigma_0 \) 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.

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

(13)

Here,

\[ I_0 = AA^* T^2 \exp \left( -\frac{q \phi_B}{K_B T} \right) \]  

(14)

Where \( I_0 \) is the reverse saturation current, \( q \) is the charge of an electron, \( V \) is the bias voltage, \( n \) is the ideality factor, \( \phi_B \) 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.

\[ n = \frac{q}{k_B T} \left( \frac{d(V)}{d(\ln(I))} \right) \]  

(15)

The effective barrier height of the Cu/Sn-WO\(_3\)/p-Si diode was calculated by the following expression.

\[ \phi_B = \frac{K_B T}{q} \ln \left( \frac{AA^* T^2}{I_0} \right) \]  

(16)

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

\[ P_s (\%) = \frac{I_{Ph} - I_D}{I_D} \times 100 \]  

(17)

\[ R = \frac{I_{Ph}}{P A} \]  

(18)

\[ QE = \frac{R \chi}{q \lambda} \]  

(19)
\[ D^* = \frac{R}{(2qI_D)^{1/2}} \]  

(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 \( \lambda \) is the wavelength.

Supplementary Figures

Fig. S1. Structural parameters vs Sn concentration (wt.%) for Sn-WO₃ films.
Fig. S2. EDX spectrum of Sn-WO₃ 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.

<table>
<thead>
<tr>
<th>Sn Concentrations (wt.%)</th>
<th>Diffraction angle 2θ (°)</th>
<th>Interplanar distance (d) (Å)</th>
<th>FWHM (Radian)</th>
<th>Crystallite size (D) (nm)</th>
<th>Micro strain (ε)</th>
<th>Dislocation density (δ) (× 10$^{14}$ lines m$^{-2}$)</th>
<th>Stacking fault (SF) (× 10$^{-2}$)</th>
<th>Texture coefficient (TC)</th>
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<td>23.34</td>
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<td>Sn concentrations (wt. %)</td>
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Table S2 Atomic percentage of Sn-WO₃ composite thin films.