

**Experiment 6: Preparation of Tin Oxide by Sol-gel Method
and its Characterization**

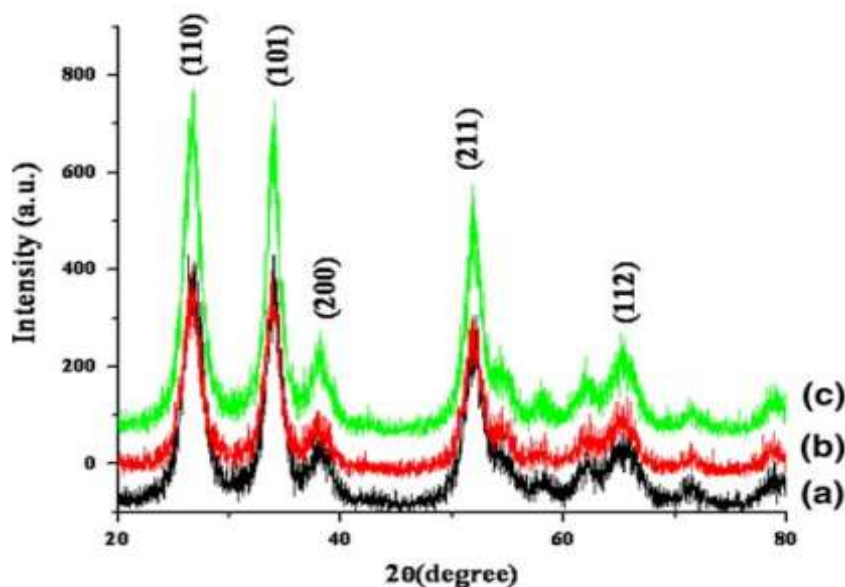
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XRD pattern of SnO₂ nanoparticles mediated in methanol (a), ethanol (b), and water (c).



Analysis:

The powder XRD peak positions for the prepared SnO₂ nanoparticles by sol-gel method are identified based on standard JCPDS file #__88-0287. This shows the tin oxide crystallizes in tetragonal crystal system **(110) peak – 27 °, (101) peak – 34 °, (200) peak – 38 °, (211) peak – 52 °, (112) peak – 65 °.**

Calculation for the determination of crystallite size of SnO₂ NPs using Scherrer's equation:

Suppose, two peaks appeared in the diffractogram as

i) (110) peak has $2\theta = 26.9169^\circ$ and $\text{FWHM} = 2.6468^\circ$

ii) (101) peak has $2\theta = 33.9169^\circ$ and $\text{FWHM} = 1.8303^\circ$

Crystallite size of SnO₂ NPs can be calculated by using Scherrer's equation as follows:

$$\boxed{\text{Crystallite size} = \frac{k\lambda}{\beta \cos\theta} \text{ nm}}$$

where, $k = 0.9$, $\lambda = 0.15406 \text{ nm}$,

β = FWHM in radian, 2θ = Bragg's angle in degree

For this calculation,

You should change 2θ to θ by dividing 2 and FWHM value in degree should be converted to radian by multiplying a factor of $\pi \times 180$.

i) for (110) peak:

$$2\theta = 26.9169^\circ,$$

$$\theta = 26.9169^\circ / 2 = 13.4584^\circ,$$

$$\cos(13.4584) = 0.972539159,$$

$$\text{FWHM} = 2.6468^\circ = 2.6468 \times \pi / 180 = 0.0461953746 \text{ radians}$$

Crystallite size = **3.086 nm**

Crystallite size = $\frac{k\lambda}{\beta \cos \theta}$ nm

where $k = 0.9$, $\lambda = 0.15406$ nm
 β = FWHM in radians
 2θ = Bragg's angle in degrees.

\therefore (i) (110) peak:

$\rightarrow 2\theta = 26.9169^\circ$
 $\Rightarrow \theta = \frac{26.9169}{2} = 13.4584^\circ$
 $\Rightarrow \cos \theta = \cos(13.4584) = 0.972539159$

$\rightarrow \text{FWHM (in degrees)} = 2.6468^\circ$
 $\Rightarrow \beta = \frac{2.6468 \times \pi}{180} = 0.0461953746 \text{ radians}$

$\therefore \cos \theta = 0.972539159$
 $\beta = 0.0461953746 \text{ radians}$

Size = $\frac{0.9 \times 0.15406}{0.0461953746 \times 0.972539159}$

$\Rightarrow \text{Size} = 3.086219512$

\therefore **Size = 3.086 nm**

ii) for (101) peak:

$$2\theta = 33.9169^\circ,$$

$$\theta = 33.9169^\circ / 2 = 16.9584^\circ,$$

$$\cos(16.9584) = 0.956516782$$

$$\text{FWHM} = 1.8303^\circ = 21.8303 \times \pi / 180 = 0.0319447613 \text{ radians}$$

Crystallite size = **4.538 nm**

(ii) (110) peak:

$$\rightarrow 2\theta = 33.9169^\circ$$

$$\theta = \frac{33.9169}{2} = 16.9584^\circ$$

$$\Rightarrow \cos\theta = \cos(16.9584) = 0.956516782$$

$$\rightarrow \text{FWHM (in degrees)} = 1.8303^\circ$$

$$\Rightarrow \beta = 1.8303 \times \frac{\pi}{180} = 0.0319447613 \text{ radians}$$

$$\therefore \cos\theta = 0.956516782$$

$$\beta = 0.0319447613 \text{ radians}$$

$$\text{Size} = \frac{0.9 \times 0.15406}{0.956516782 \times 0.0319447613}$$

$$\Rightarrow \text{Size} = 4.53774578$$

$$\therefore \boxed{\text{Size} = 4.538 \text{ nm}}$$

Result:

(i) The powder XRD peak positions for the prepared by SnO₂ nanoparticles are:

- a. (110) peak – 27°**
- b. (101) peak – 34°**
- c. (200) peak – 38°**
- d. (211) peak – 52°**
- e. (112) peak – 65°**

(ii) Particle size/ crystallite size:

- a. (110) peak – 3.086 nm**
- b. (101) peak – 4.538 nm**