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# Preparation of $TiO_2$ nanopowder depicting lower energy band gap for solar and gas sensing applications

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**Abstract**
*$TiO_2$ nanopowder exhibiting pure anatase and rutile phase are prepared by simple sol gel method after annealing at $500^0C$ and $900^0C$ for 1 hour in air respectively. X-ray diffraction pattern (XRD) is used to calculate crystallite size by Scherrer's formula as 15±5 nm for $TiO_2$-$500^0C$ and 25±5 nm for $TiO_2$-$900^0C$ nanopowder. UV spectrometer is used to obtain Tauc's plot in order to calculate energy band gap values. It is observed that energy band gap values of prepared $TiO_2$-$500^0C$ and $TiO_2$-$900^0C$ nanopowder are less as compared to pure anatase phase energy band value 3.2 eV and pure rutile phase 3.0 eV. Therefore the reduced energy band gap values of prepared $TiO_2$-$500^0C$ and $TiO_2$-$900^0C$ nanopowder enhances its suitability in the field of solar energy and gas sensing.*

**Keywords:** *anatase, rutile, band gap, nanopowder.*

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## I. INTRODUCTION

Titanium dioxide ($TiO_2$) plays significant role in the field of material science and nanotechnology. It exhibits high stability against corrosion, self cleaning with strong oxidation stability as well as excellent optical properties. $TiO_2$ is extensively used in solar cells, photocatalysis, hydrogen storage and gas sensors [1-5]. It exists in three polymorphs anatase, rutile and brookite. The anatase form of $TiO_2$ shows large energy band gap of 3.2 eV and energy band gap value of rutile phase corresponds to 3.0 eV [6]. The energy band gap value of $TiO_2$ indicates that it cannot observe visible light efficiently. Therefore it is highly desirable to prepare $TiO_2$ which yields lower energy band gap [7].

Several methods have been established for the preparation of $TiO_2$ such as sol-gel method, chemical vapour oxidation method, hydrothermal method, oxidation method and many more [8-10]. Sol-gel method is one of the most widely used techniques due to its possibility of evolving unique metastable structure at low temperature with excellent homogeneity [8]. Hence in our present investigation we use sol-gel method to prepare $TiO_2$ nanopowder at $500^0C$ and $900^0C$ with a reduced energy band gap value.

## II. EXPERIMENTAL

Sol-gel method is employed to prepare $TiO_2$ nanopowder. The AR grade chemicals used are titanium isopropoxide (TTIP) and methanol. A solution is prepared by using 3.5 ml TTIP and 40 ml methanol in a beaker. This solution is milky white in colour and it is stirred for 1:30 hours at a temperature of $57±3^0C$ using magnetic stirrer. The gel obtained is kept for 12 hours at room temperature [11]. The powder thus obtained is collected and annealed at $500^0C$ and $900^0C$ for 1 hour in air respectively. X-ray diffraction technique (XRD) and UV-spectrometer is used to characterize the prepared $TiO_2$ specimens.

## III. RESULTS

X-ray diffraction pattern of $TiO_2$ nanopowders annealed at $500^0C$ and $900^0C$ are recorded using $CuK_\alpha$ radiation as shown in Fig. 1. The crystallite size is calculated by Scherrer's formula [12]:

$$D = 0.89\,\lambda / \beta \cos\theta \qquad (1)$$

where D is crystallite size in nanometer, β is the full width at half maximum (FWHM) in radian, λ is the wavelength of the X-ray which is 0.15406 nm for Cu target Kα radiation and θ is the Bragg angle.

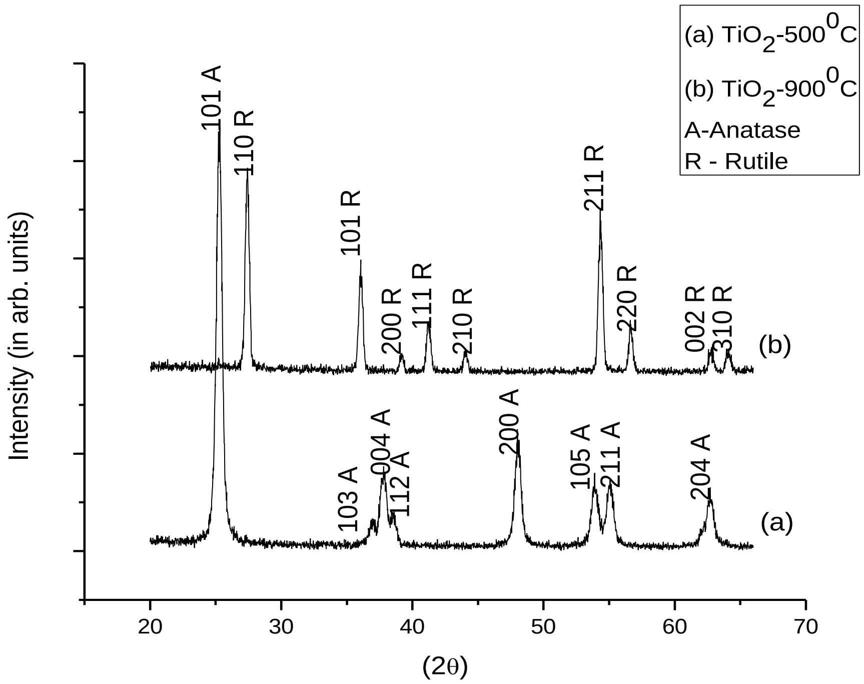


**Figure1: X-ray diffraction pattern of $TiO_2$ nanopowder annealed at (a) $500^0$C and (b) $900^0$C.**

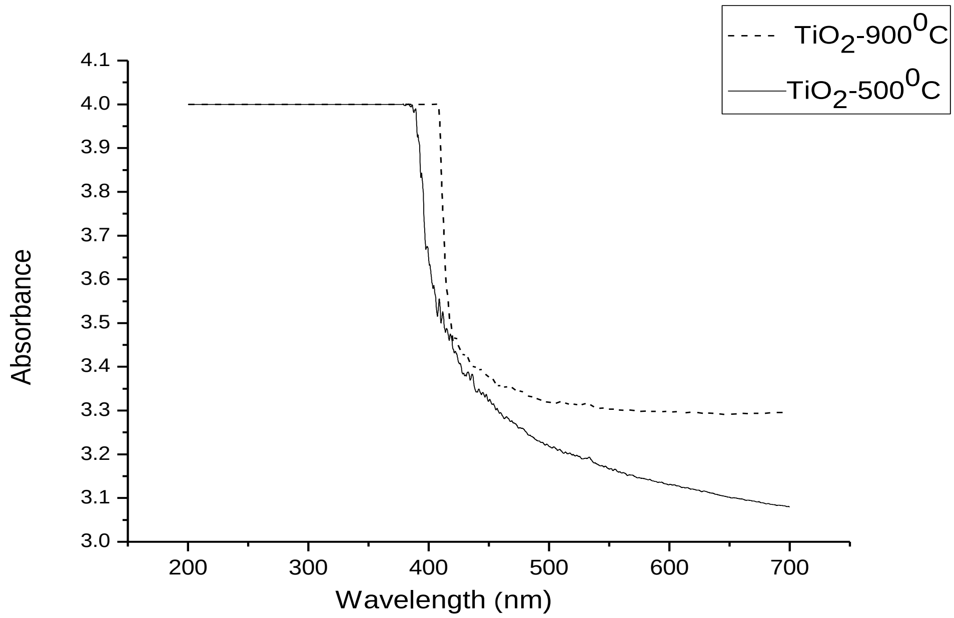


**Figure 2: UV spectra of $TiO_2$ nanopowder annealed at $500^0$C and $900^0$C.**

Fig. 2 shows UV spectra of $TiO_2$-$500^0$C and $TiO_2$-$900^0$C specimen recorded at Shimadzu UV-1800. The data is used to obtain Tauc plots as shown in Fig. 3 [4, 13]. The energy band gap values calculated using Tauc's plot and average crystallite size obtained by Scherrer's formula is mentioned in Table 1.

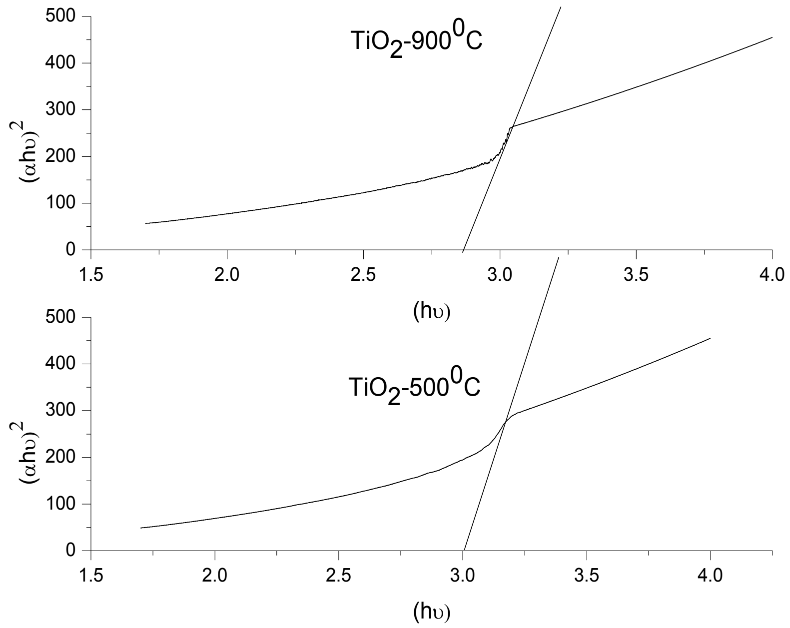


**Figure 3: Tauc plot of $TiO_2$ nanopowder to calculate energy band gap value.**

**Table 1: XRD and UV results of $TiO_2$ nanopowder annealed at $500^0$C and $900^0$C.**

| S.No. | Specimen | Average Crystallite Size | Energy Band Gap (eV) |
|---|---|---|---|
| 1 | $TiO_2$-$500^0$C | 15±5 nm | 3.00 |
| 2 | $TiO_2$-$900^0$C | 25±5 nm | 2.87 |

## IV. DISCUSSION

X-ray diffraction pattern depicts peaks of pure anatase phase for $TiO_2$-$500^0$C specimen and peaks of pure rutile phase for $TiO_2$-$900^0$C specimen. The diffraction angles are in good agreement with JCPDS no 21-1272 for anatase, JCPDS no 21-1276 for rutile and data reported in the literature [4, 12]. It is also observed that average crystallite size increases with increase in annealing temperature.

The energy band gap values of $TiO_2$-$500^0$C and $TiO_2$-$900^0$C nanopowder obtained by Tauc plot is lower as compared to anatase phase 3.2 eV and rutile phase 3.0 eV [6, 7]. It is also observed that energy band gap value decreases with increase in annealing temperature. Therefore the optimised preparation method of $TiO_2$ nanopowder leads to lower energy band gap values and lower average crystallite size. Hence the prepared $TiO_2$ nanopowders annealed at $500^0$C and $900^0$C may exhibit a potential candidate in the field of solar cell and gas sensing [14, 15].

## V. CONCLUSION

1. The lower energy band gap values of $TiO_2$ nanopowder increases its suitability for solar and gas sensing applications.
2. $TiO_2$ nanopowder annealed at $500^0$C and $900^0$C depicts pure anatase and pure rutile phase respectively.


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