



## TRANSITION MODEL ANALYSIS OF BISMUTH OXIDE QUANTUM DOTS

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### ABSTRACT

The bismuth oxide is very stable metal oxide with wide range of applications. The bismuth oxide quantum dots (QDs) were arrested through chemical method. The  $\text{Bi}_2\text{O}_3$  QDs were prepared by varying bismuth nitrate (0.25-1M) in constant 1M hexamethylenetetramine. The samples were characterized by UV-Vis analysis. Quantum size effect where the electronic and optical properties of solids are altered due to changes in the band structures. This change in band structure studied by means of UV spectroscopy using transition probability model. The highest value of optical band gap was found to be 4.5 eV at 0.5M concentration of bismuth nitrate where as smallest QDs radius 2.56 nm also found for same concentration.

**Key words:** Transition Probability Model, Bismuth oxide, Quantum Dots.

### INTRODUCTION

The metal oxides have been attracted great attention due to ease of synthesis, less toxic, reliability, cheaper etc. Amongst them, bismuth oxide has been mainly used in many application such as photochemical solar cells, varistors, gas sensors, pharmaceutical & metallurgical additives etc. Up till now five polymorphic forms were found for  $\text{Bi}_2\text{O}_3$ , each of them with its specific properties: two stable polymorphs namely  $\alpha$  &  $\delta$  ( $\alpha$ -  $\text{Bi}_2\text{O}_3$  is monoclinic.  $\delta$ - $\text{Bi}_2\text{O}_3$  is face centred cubic) & three metastable phases,  $\gamma$  &  $\omega$  respectively ( $\beta$ -  $\text{Bi}_2\text{O}_3$  is tetragonal;  $\gamma$ -  $\text{Bi}_2\text{O}_3$  is body centre cubic,  $\omega$ -  $\text{Bi}_2\text{O}_3$  is triclinic)<sup>1</sup>.  $\text{Bi}_2\text{O}_3$  is also used as an additive in paints.

The advantageous analytical properties of bismuth are attributed to its fused alloy formation with different metals<sup>2-4</sup>. Semimetal bismuth, which has a highly anisotropic Fermi surface, low conduction band effective mass and high electron mobility is of great interest because of its size induced semimetal to semiconductor transition<sup>5-8</sup>. When crystallite size is decreased to nano scale, semimetal bismuth is converted to a semiconductor due to quantum confinement effect, this makes bismuth nanoparticles especially useful for optoelectronic & thermoelectric application.

Crystalline bismuth oxide is prepared by conventional high temperature solid state reaction of bismuth salts<sup>9</sup> or by means of mechanochemical synthesis<sup>10,11</sup>. Non-conventional method such as

hydrothermal synthesis<sup>12</sup> and sonochemical synthesis<sup>13</sup> are also used for bismuth oxide preparation. However most of the methods are based on precipitation reaction of bismuth salts and calcinations of bismuth products nucleation and growth of particles in a course of hydrolysis or condensation of bismuth salts can be controlled by means of additives such as polyethylene, polyvinylpyrillidon, urea and/or citric acid<sup>14-20</sup>.

In the present work, Bi<sub>2</sub>O<sub>3</sub> nanoparticles were synthesized by single step chemical method with different concentration of bismuth nitrate in HMT as a nitrate remover at room temperature. The samples were characterized by UV-VIS analysis to know the particle size.

## EXPERIMENTAL

### Synthesis of Bi<sub>2</sub>O<sub>3</sub> nanoparticles

Bismuth nitrate & hexamethylenetetramine used for the preparation of Bi<sub>2</sub>O<sub>3</sub> were of AR grade (SD fine, India). A known quality of (1M= 4 .85 g) of Bi (NO<sub>3</sub>).5H<sub>2</sub>O mixed with (1 M) HMT dissolved in 30ml water. The mixture stir with magnetic stirrer for 15 min. Various samples of bismuth oxide were prepared by varying concentration of bismuth nitrate (such as 0.25%, 0.50%, 0.75%, 1 M) in 1 M constant HMT. Optical absorption studies were carried out using UV-VIS spectrometer (Perkin Elmer) in wavelength range 350-550 nm.

## RESULTS AND DISCUSSION

The UV-vis analysis was carried out to know the optical properties of prepared samples. The particle size of the samples was estimated roughly from optical band gap value. The UV-vis spectra of samples were displayed in Fig. 1. This analysis provides optical information of synthesized materials.

By considering shifted absorption edge from 275-364 nm of Bi<sub>2</sub>O<sub>3</sub> sample

$$R = \sqrt{\frac{2\pi^2 h^2 E_{bulk}}{m^* (E_{nano}^2 - E_{bulk}^2)}} \quad \dots(1)$$

where,  $E_{bulk}$  is bulk band gap ( $E_{bulk} = 2.85$  eV)

$E_{nano}$  is band gap of nanomaterial,

$m^*$  is effective mass of electron ( $m^* = 29.15 \times 10^{-31}$  Kg)

The plot between concentrations of bismuth nitrate versus optical band gap shown in fig.2 reflect optical band gap highest for 0.5M concentration of bismuth nitrate. The quantum dot radius found to be smallest for same concentration of bismuth nitrate shown in fig.3, which excellently collaborates with theoretical interpretation.

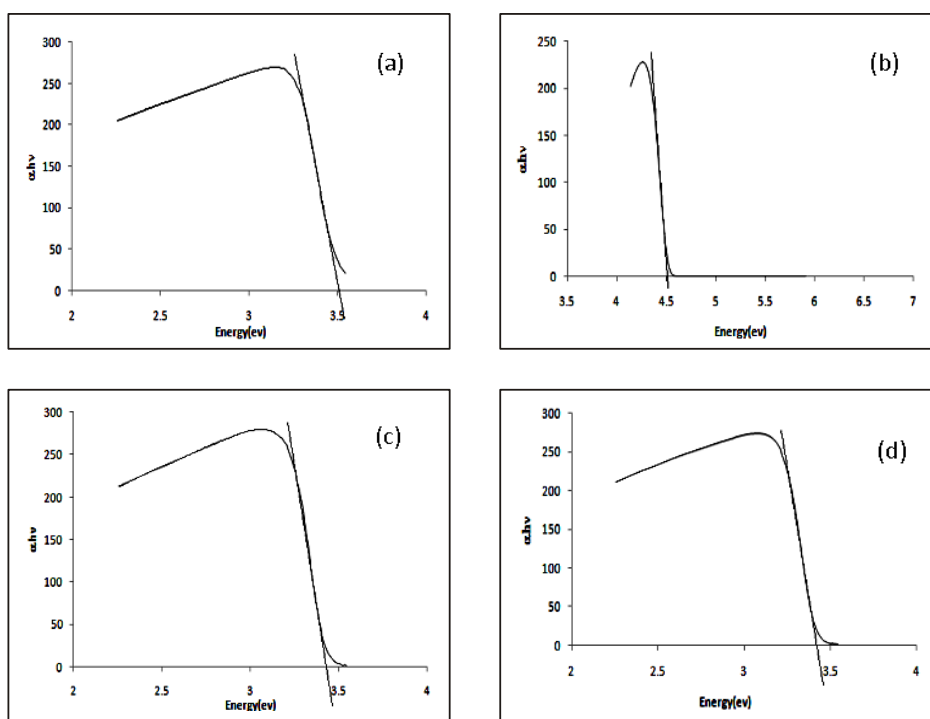
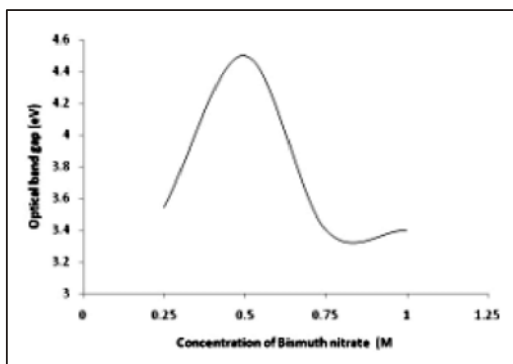
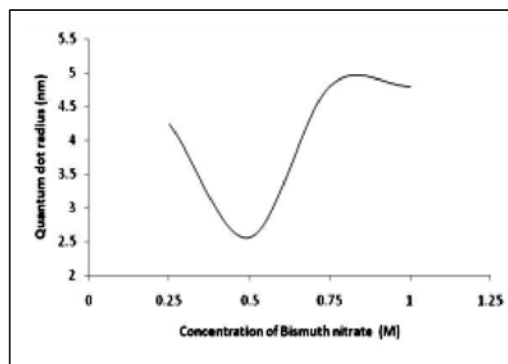
### Transition probability Model

Optical band gap analysis of prepared Bi<sub>2</sub>O<sub>3</sub> QDs were done through Fermi's golden rule using eq.1. The computed value of optical band gap enlisted in Table 1.

$$E \text{ (eV)} * \lambda \text{ (\mu m)} = 1.24 \quad \dots(2)$$

**Table 1: Values of Absorption wavelength, Optical band gap and Quantum dot radius (R) for different concentration of bismuth nitrate**

| S. No. | Molar concentration of bismuth nitrate | Absorption wavelength (nm) | Optical band gap (eV) | Quantum dot radius (R) (nm) |
|--------|--|----------------------------|-----------------------|-----------------------------|
| 1      | 0.25                                   | 350                        | 3.54                  | 4.24                        |
| 2      | 0.50                                   | 275                        | 4.50                  | 2.56                        |
| 3      | 0.75                                   | 364                        | 3.40                  | 4.80                        |
| 4      | 1                                      | 364                        | 3.40                  | 4.80                        |

**Fig. 1: Variation of  $\alpha h\nu$  with energy for (a) 0.25 M, (b) 0.5 M, (c) 0.75 M and (d) 1 M bismuth nitrate****Fig. 2: Plot between concentration of Bismuth nitrate versus optical band gap****Fig. 3: Plot between concentration of Bismuth nitrate versus quantum dots radius**

## CONCLUSION

The UV spectroscopy is very simple technique for optical study of materials. UV-vis study reveals that at 0.5 M concentration of bismuth nitrate showed maximum value of band gap 4.5 eV. The quantum dot radius was found to be smallest for same concentration.

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