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OPTICAL PROPERTIES STUDY OF NANOSTRUCTURED CeO_2 USING HYPERBOLIC BAND MODEL

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ABSTRACT

Quantum size effect where the electronic and optical properties of solids are altered due to changes in the band structures, enhanced the surface/volume ratio in nano dimensions forces more than 33% of the atoms to be on the surface (for 10 nm dot 35), which drastically altering the physical properties. Consequently, optical study becomes crucial. CeO_2 is an important rare earth metal oxide with the basis of several potential applications and implications. Nanostructured CeO_2 was synthesized through single step chemical rout method. In present investigation, optical Band Gap and transition probability studied from UV spectrophotometer.

Key words: Optical properties, CeO_2, Hyperbolic band model.

INTRODUCTION

CeO_2 is a useful industrial material for applications such as solid state electrolytes for electrochemical devices as well as oxygen storage capacity component in three way automotive catalyst[1-4]. Optical band gap of CeO_2 is 1.85 eV at bulk level. CeO_2 is a wide band gap semiconductor that has long been known for its catalytic capabilities[5] and has been synthesize and studied in both thin film[6,7] and nano particle form[8-10]. As a thin film CeO_2 has unique properties such as a high refractive index, a high dc dielectric constant and a lattice constant similar to Si, making it suitable as insulating material in Si device technology[11]. These properties make CeO_2 useful for applications in microelectronics and optics.

Recently, ceria nano particles have attracted attention within the biomedical community as a potential agent to inhibit cellular aging[12,13]. Mixed brain cell cultures have been shown to have an increased lifespan when a solution containing ceria nano particles is introduced into their environment. CeO_2 was chosen because it may act as a free radical scavenger. CeO_2 is used in ceramics, to sensitize photosensitive glass, as a catalyst and as a catalyst support, to polish glass and stones, in lapidary as an alternative to "jweller's rouge". It is also known as "optician's rouge'. It is also used in the walls of self cleaning ovens as a hydrocarbon catalyst during the high temperature cleaning process. While it is transparent for visible light, it absorbs ultraviolet radiation strongly, so it is a prospective replacement of zinc oxide and titanium dioxide in sunscreens, as it has lower photocatalytic activity. However its thermal catalytic properties have to be

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decrease by coating the particles with amorphous silica or boron nitride. The use of these nano particles, which can penetrate the body and reach internal organs, has been criticized as unsafe[14].

In this present article, synthesis of CeO_2 nano particles synthesized through chemical single step method by varying concentration of hexamethylenetetramine (HMT) in constant 1M cerous nitrate at room temperature. Materials were characterized by UV-visible spectrophotometer.

EXPERIMENTAL

AR grade (SD fine, India) chemicals were used in present work. The CeO_2 was synthesized by single step chemical method. The hexamethylele tetramine (HMT) with different concentration (0.25-1 M) was dissolved in 5 ml double distilled water separately. After rigorous stirring, 1 M cerous nitrate was added in the solution. The reaction was stand for 4 h. The precipitate so obtained was vacuum filtered and filtrate was first dried at room temperature of 24 h and sintered at 100°C for 3 h. In this way, four samples of CeO_2 were prepared. The samples were characterized by UV-Vis analysis on Perkin Elmer Spectrophotometer.

RESULTS AND DISCUSSION

Optical band gap analysis with hyperbolic band model

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 using hyperbolic band model. The UV-vis spectra of samples were displayed in Fig. 1, 2, 3, 4. This analysis provides optical information of synthesized CeO_2 sampels. Using various models regarding the optical properties can apply to this data, gives very interesting result. In our present investigation we apply hyperbolic band model to study the optical properties of prepared samples and the particle size also computed from same model.

Table 1: Values of absorption wave length, optical band gap and quantum dot radius (R) of CeO_2 of different concentration of HMT

S. No.	Sample	Optical band gap (eV)	Quantum dot radius (R) nm
1	0.25 M HMT	3.25	2.77 nm
2	0.50 M HMT	3.41	2.91 nm
3	0.75 M HMT	3.40	2.59 nm
4	1 M HMT	3.41	2.58 nm

By considering shifting in absorption edge towards lower wavelength in CeO_2 samples, average crystallite (particle) size has been estimated by using the hyperbolic band model[154].

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

where, E_{bulk} is bulk band gap, E_{nano} is band gap of nanomaterial, m* is effective mass of electron ($m^*=29.15 \times 10^{-31}$ Kg).

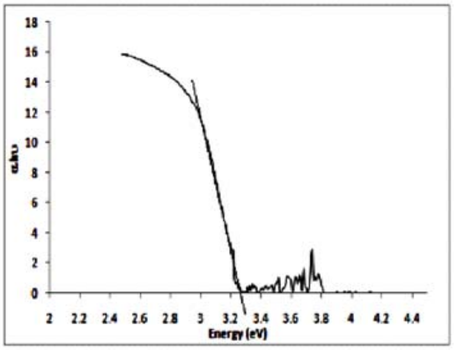

Fig. 1: UV-Vis of 0.25 M HMT

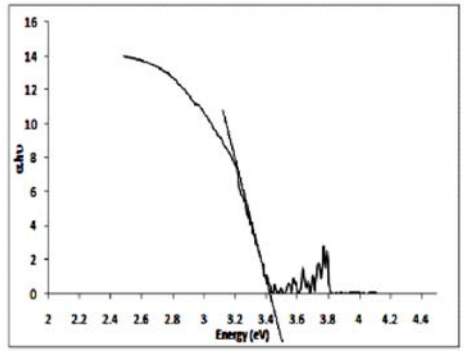

Fig. 2: UV-Vis of 0.5 M HMT

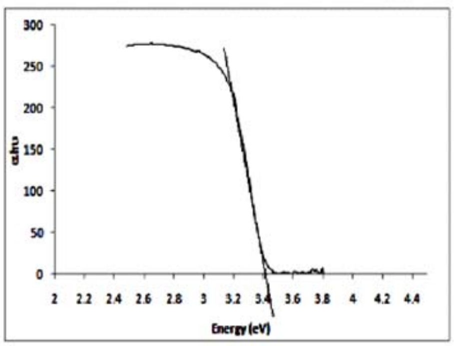

Fig. 3: UV-Vis of 0.75 M HMT

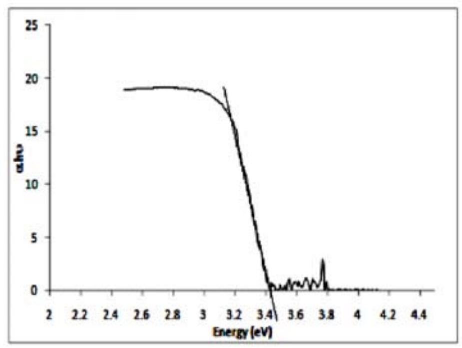

Fig. 4: UV-Vis of 1 M HMT

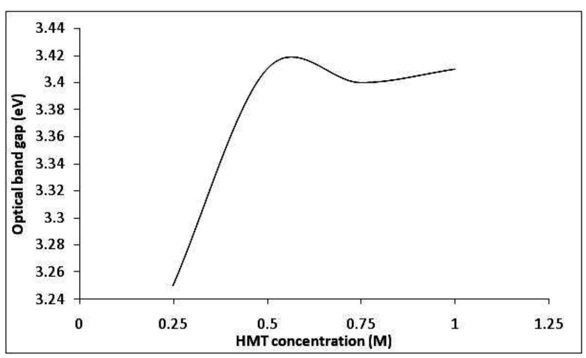

Fig. 5: Plot between HMT concentration versus optical band gap

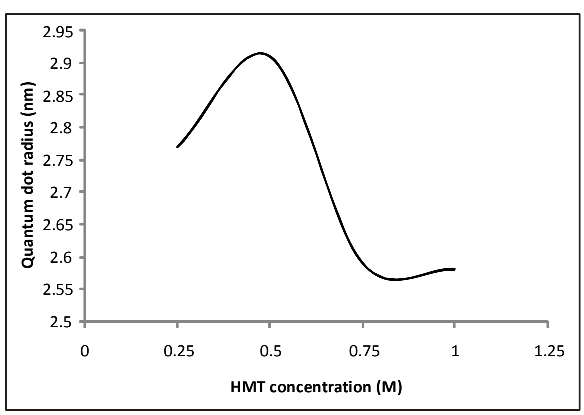

Fig. 6: Plot between HMT concentration versus quantum dot radius (nm)

CONCLUSION

Chemical synthesis of CeO_2 nanoparticals is a simple, low cost and reliable technique. UV-vis study revels that the as concentration of HMT increases band gap of samples also increase. The value of band gap increased to a maximum at ~ 0.5 M concentration of HMT. The quatum dot radius was found to be small at 1 M HMT concentration.

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