Nano Crystalline SnO$_2$: An Alternative Method for Experimental Estimation of Reduced Effective Mass of Excitons

Mohsen Dehbashi* and Seyed Javad Hosseini
Department of Physics, Sciences Faculty, University of Zabol, Zabol, Iran; Mohsendehbashi.mdb@gmail.com, s.javad.hosseini12@gmail.com

Abstract

Background: In this work, SnO$_2$ nanoparticles were successfully prepared by using Co-precipitation route, from hydrous SnCl$_2$.2H$_2$O (98% Merck) using aqueous ammonia, this method found to be very facile and cost-effective. Methods: The samples characterized by various techniques such as, TEM, XRD and UV–Vis spectroscopy. In this paper, an alternative way presented for experimental estimation of reduced effective mass of exciton for semiconductor nanoparticles. Results: A semiconductor nanoparticle obtained from UV-visible spectrum and uses the effective mass approximation model, which related the energy band gap to the reduced effective mass of exciton ($\mu$) and size of nanoparticles (R). In this paper, SnO$_2$ nanoparticles that are semiconductors are chosen for size estimations. The UV-visible spectrum shown that wavelength of edge has been occurred in 344.5 nm. The reduced effective mass of exciton acquired 2.495 X 10$^{-31}$ Kg, using the effective mass approximation model. Conclusion: The results of this study are in well concurrence with results that are obtained from literatures.

Keywords: Alternative Method, Exciton, Nano Crystalline, Reduced Effective Mass, SnO$_2$

1. Introduction

In solid-state physics, effective mass of particle, mass is that it seems to have when moving in solid and affected by various forces. The effective mass is main parameter that influences properties of a material. For many solids, the effective mass consider as simple constant of solid. In this paper, we want to estimation the reduced effective mass of exciton, which is remarked in the term of effective mass of hole and electron. Many theoretical models have been suggested to explain the relationship between reduced effective mass of exciton and particles size$^{1-3}$. For this work, the Effective Mass Approximation (EMA) model was selected to estimation of reduced effective mass of exciton, which is most used model, proposed by$^4$.

2. Experimental Methods

SnO$_2$ nanoparticles were synthesized with precipitation of hydrous SnCl$_2$.2H$_2$O (98% Merck) using aqueous ammonia, this method found to be very facile and cost-effective. Crystallinity, structure and average size of SnO$_2$ nanoparticles were obtained by means of X-Ray Diffraction (XRD) using Rigaku-Miniflex X-ray. The morphology and dimensions of SnO$_2$ nanoparticles were obtained with a Hitachi H-800 Transmission Electron Microscope (TEM) and UV-Vis transmittance spectrum of the nanoparticles was obtained by means of PG instrument T80 UV-Vis spectrophotometer.

3. Results and Discussion

In the effective mass approximation model, semiconductor nanoparticles considered as a sphere having radius of R, with an infinite potential barrier at the boundaries. When the electrons and holes (excitons) in particles are confined to nanometer dimensions, they are closer together and the Coulombic interaction between them cannot anymore be neglected. For such systems, dependence of energy band gap on size and exciton effective
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Mass could be accurately calculated by following equation$^4$,

$$E_g - E_{g, \text{bulk}} = \frac{\hbar^2 \pi^2}{2R^2} \left( \frac{1}{m^*_e} + \frac{1}{m^*_h} \right) - \frac{1.786e^2}{\varepsilon R}$$  \tag{1}

Where $E_g$ is the energy band gap of nanoparticles, $E_{g, \text{bulk}}$ is the energy band gap of bulk semiconductor. $R$ is the size of nanoparticle, $m^*_e$ and $m^*_h$ are the hole and electron effective mass respectively, $\varepsilon$ is the permittivity of the semiconductor material and $\hbar$ is in the plank's constant. The first term in Equation 1 describes the kinetic energy of exciton and the second term is due to Coulomb interaction energy in exciton. This paper consists of three parts. First determination of the size of SnO$_2$ nanoparticles with the X-ray diffraction spectrum, TEM photograph use to show that nanoparticles have spherical shape. Second calculation of energy band gap of semiconductor nanoparticles with the UV-visible spectrum. Finally, applying the Bruce model to determination of the exciting effective mass for SnO$_2$ nanoparticles.

$\text{Figure 1. X-ray diffraction plot of SnO}_2$ nanoparticles.

3.1 Determination of Size and Morphological Properties of SnO$_2$ Nanoparticles

Crystalline structure of the SnO$_2$ nanoparticles acquired by X-ray diffraction is shown in Figure 1. The X-ray diffraction pattern of SnO$_2$ nanoparticles show three stronger peaks at 26.7, 33.8 and 51.8 (2θ) and eight weaker peaks at 38.1, 54.8, 57.9, 61.8, 64.6, 65.8, 71.1, 78.9 (2θ), demonstrating the formation of tetragonal phase of the SnO$_2$ nanoparticles. The average crystalline size of nanoparticles found to be 19.02 nm by means of Scherer formula.

$\text{Figure 2 shows TEM photograph of SnO}_2$ nanoparticles which have nearly spherical shape and uniform in size.

$\text{Figure 2. TEM photograph of SnO}_2$ nanoparticles.

3.2 Estimation of Energy Band Gap of the Nanoparticles

Figure 3 shows the optical absorbance of SnO$_2$ nanoparticles as a function of wavelength in the UV-visible range. In this section, we find the energy band gap $E_g$ of the nano crystals from the UV-visible spectrum. Energy band gap of sample could be estimated by finding the absorption edge on the wavelength axis ($\lambda_g$) in UV-visible spectrum, and using following formula,

$$E_g = \frac{hc}{\lambda_g}$$  \tag{2}

Where, $h$ (plank's constant) and $c$ (speed of light) are equal to 6.626 X 10$^{-34}$ Js and 2.9979 X 10$^8$ ms$^{-1}$ respectively. As showing Figure 3, absorption edge occurs in wavelength of 344.5 nm. The wavelength of edge was estimation by extrapolating the horizontal and vertical portions of the curve and defining the edge as the wavelength of the intersection $\lambda_g$. Thus, the energy band gap of sample was calculated$^2$ as 3.6038eV from Equation 2.

3.3 Estimation of Reduced Effective Mass of Exciton in SnO$_2$ Nanoparticles

When size of the particles approach to the nano dimensions, a blue shift in energy is observed due to the quantum confinement phenomenon. In order to study the size dependence of optical properties of systems, two confinement regimes are defined: weak and strong confinements. In the weak confinements, the particle size is larger than...
Bohr radius \( a_B \) and the electron and the hole are treated as a correlated pair. The blue shift could be perceived by considering only first term of Equation 1.

\[
\Delta E_g = \frac{\hbar^2 \pi^2}{2R^2} \frac{1}{\Delta E_g}
\]

Where \( \Delta E_g = E_g - E_{g, \text{bulk}} \) and \( E_{g, \text{bulk}} = 3.6 \text{ eV} \) for Tin dioxide in bulk phase, \( R \) and \( \Delta E_g \) determined in previous parts.

By substituting these values in Equation 3, the reduced effective mass of exciton acquired 2.495 \( \times 10^{-31} \text{ Kg} \). This is well-agreeing with the reported literatures.

### 4. Summary and Conclusion

The SnO\(_2\) nano crystals have been facilely synthesized by co-precipitation method. We present an alternative method for experimental estimation of reduced effective mass of exciton. The wavelength of edge occurred in 344.5 nm. The reduced effective mass of exciton acquired using the effective mass approximation model was 2.495 \( \times 10^{-31} \text{ Kg} \). This is in well concurrence with results that are obtained from the literature.

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