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Synthesis of ZnO Nanopowder by using Sol-Gel and Theoretical Study of Brus Equation

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Abstract

Zinc oxide (ZnO) nanoparticles are a marvel in nanotechnology, celebrated for their extraordinary properties and adaptability across diverse fields. Their nanoscale size and high surface area-to-volume ratio endow them with distinct chemical and physical characteristics, making them indispensable in cutting-edge technological advancements.

Crafting ZnO nanoparticles is an art that involves methods ranging from chemical vapour deposition to sol-gel techniques. Each method holds unique advantages in controlling particle size the purity, and scalability. Sol-gel method synthesis technique utilized zinc acetate dihydrate as a precursor, while potassium hydroxide was employed to maintain precise pH control. The nanoparticles underwent controlled thermal processing initially at 80^{o}C and followed by annealing at 200^{o}C to enhance the stability and optimize quantum effect. UV-vis spectroscopy indicated a distinct absorption peak at 367.8 nm, corresponding to a band gap of 3.37 eV which confirms quantum confinement induced energy level. Utilizing Brus equation alongside effective mass approximations, the estimated particle radius was found to be approximately 4.06 nm ensuring strong excitonic interaction due to spatial wave function overlap.

Keywords - *ZnO Nanoparticle, Sol-gel Method, UV-Vis spectroscopy, Brus equation.*

Introduction

A critical aspect of understanding the optical properties of ZnO nanoparticles lies in the quantum size effect, which significantly influences their behaviour at the nanoscale. This is where the Brus equation comes into play. The Brus equation provides a quantitative framework for analyzing the quantum confinement effects in semiconductor nanocrystals, such as ZnO nanoparticles.

The Brus equation is given by:

$$E = E_g + \frac{\hbar^2 \pi^2}{2R^2} \left\{ \frac{1}{m_e} + \frac{1}{m_h} \right\} - \frac{1.8e^2}{4\pi\varepsilon_0 R}$$

Where,

E is the band gap of the synthesized particle, Eg the bulk band gap of ZnO (3.3eV),R radius of the particle, me effective mass of the electron (for ZnO, it is 0.28m0), mh effective mass of hole (for ZnO it is 0.49m0), ε - dielectric constant of material (for ZnO it is 9.1), εo permittivity of free space and h is the Planck’s constant

This equation illustrates how the band gap energy of ZnO nanoparticles increases as their size decreases due to the quantum confinement. The insights provided by the Brus equation are crucial for tailoring the optical properties of ZnO nanoparticles to specific applications, such as in optoelectronics and photonics. By understanding the principles behind the Brus equation, researchers can better design and optimize the synthesis processes to achieve ZnO nanoparticles with desired properties. This not only enhances the functionality of the nanoparticles but also broadens their applicability in various technological domains.

Sol-gel Technique

The sol-gel technique is a versatile method for producing ceramic and glass materials, including nanoparticles like ZnO, The process involves transitioning from a liquid "sol" into a solid "gel" phase. This process starts with the preparation of a solution containing metal precursors, which undergo hydrolysis and polycondensation to form a gel network. The gel is then dried to remove solvents and is often subjected to heat treatment (calcination) to produce the final oxide material with the desired properties.

The sol-gel method is praised for its ability to produce uniform and high-purity materials at relatively low temperatures, making it ideal for various advanced applications in nanotechnology. Parameters decided as follows:

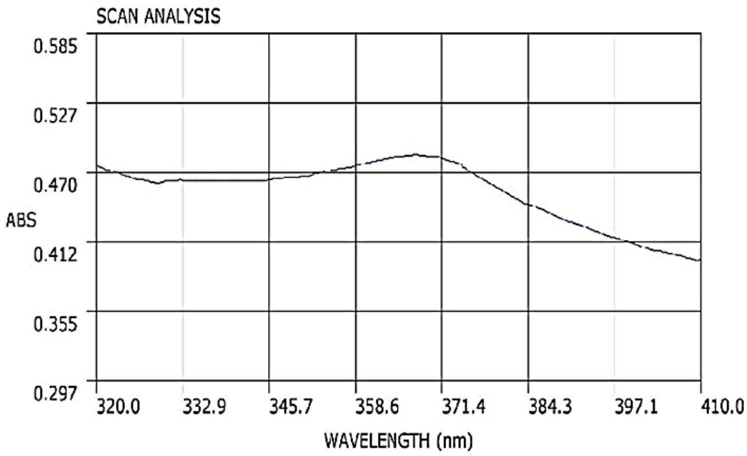
- Precursor Concentration: The concentration of zinc precursor (zinc acetate) affects the particle size and morphology.
- pH Value: Adjusting the pH using a base (potassium hydroxide) helps control the nucleation and growth of nanoparticles.
- Reaction Time: The duration of the hydrolysis and condensation reactions influences the particle size and crystallinity.
- Temperature: The calcination temperature during the drying process affects the crystalline structure and phase purity of the nanoparticles.
- Stirring Rate: Proper mixing ensures uniform distribution of reactants and uniform particle size.
- Solvent Type: The choice of solvent can impact the solubility of precursors and the overall reaction kinetics.
- Chemicals Used: Zinc acetate dihydrate, Ethanol, Potassium hydroxide (KOH), Citric acid, Dimethyl sulfoxide (DMSO), Distilled water

Procedure

1. Preparation of Zinc Solution: Dissolved zinc acetate dihydrate in ethanol.
2. Adding Citric Acid: Citric acid, was mixed and stirred continuously.
3. Adjustment of pH: Slowly KOH solution was added until pH reaches around 10, ensuring proper nanoparticle formation.
4. Forming Sol: The mixture was stirred for 2 hours to create a stable sol.

5. Adding DMSO: DMSO was incorporated to stabilize and uniformly distribute the nanoparticles.
6. Gelation: Allowed the sol to age at room temperature for 24 hours to form a gel.
7. Drying: Dried the gel at 80°C for 12 hours.
8. Calcination: Calcinated the dried gel at 200°C for 2 hours to obtain ZnO nanoparticles.
9. Characterization: Analysed the nanoparticles using UV-Vis spectroscopy.

After analysing the prepared ZnO Nanoparticles using UV-Vis Absorption Spectroscope following graph is obtained:



The graph shows a peak value at a wavelength of approximately 367.8 nm, with an absorbance (ABS) of 0.485.

Using this we can calculate the band gap energy: E = hc/ λ
E = (6.67 *10-34 * 3 *108) / (367 *10-9) = 5.4
*10-19 J = 3.37 eV

This is used to determine the average particle size using effective mass approximation. And now, Using the Brus Equation

$$E = E_g + \frac{\hbar^2\pi^2}{2R^2}\left\{\frac{1}{m_e} + \frac{1}{m_h}\right\} - \frac{1.8e^2}{4\pi\varepsilon_0 R}$$

E = 3.37 + h2π2/2R2(1/0.23me + 1/0.49mh) – 1.8 *(1.6*10-19)2/4π εoR
Therefore, R = 4.06 nm

Results

Thus, it is confirmed that the prepared ZnO nanoparticles by the sol gel method of at temperature is of size 4.06nm.

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