

## Structural, Morphological And Optical Properties Of Hydrothermally Synthesized CdS Nanoparticles

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**ABSTRACT:** CdS nanoparticles have been synthesized via a hydrothermal method using cadmium nitrate and sodium sulfide as a cadmium and sulfur ion sources. The reaction was carried out at 180 °C for 24 h. The as-prepared sample was characterized by several techniques such as X-ray diffraction (XRD), scanning electron microscopy (SEM) along with energy-dispersive X-ray spectroscopy (EDAX), UV-vis absorption spectroscopy and photoluminescence spectroscopy. The X-ray diffraction (XRD) study and relevant analysis confirmed the well crystalline hexagonal structure of CdS product with lattice constants,  $a = 4.106 \text{ \AA}$  and  $c = 6.680 \text{ \AA}$ . The morphological study reveals that CdS nanoparticles exhibit spherical granules structure. The optical band gap energy of the synthesized sample was found to be 2.47 eV. The photoluminescence spectrum showed a sharp and narrow emission peak at 524 nm.

**Keywords:** Cadmium sulfide, hydrothermal route, nanoparticles, optical properties

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### I. INTRODUCTION

Since the 21 century, group II-VI nanomaterial's have expanded its applicability due to their enhanced structure, size and optical properties and a huge potential development of process phenomena to various fields including nanoelectronics, optoelectronics, bio-related fields, semi-conducting devices[1-5].

Among these various nanomaterials, cadmium sulfide (CdS), with a direct band gap of 2.4 eV at room temperature and has attracted tremendous interest due to it has attractive physicochemical properties, special orientation and arrangement[6-7]. This material has immense potential applications in photoconductive optical switches, nanogenerators, solar cell, light emitting diodes and electro – optic modulator[8-10].

A variety of methods can be used for the formation of CdS nanoparticle that includes chemical bath deposition, electrochemical deposition, sol-gel synthesis, hydrothermal route and solvothermal method [11-15]. Among these methods hydrothermal method appears to be practical, convenient, cost effective approach to synthesis the CdS nanoparticles because it does not involve any special instrumentation and growth rate can easily control.

In this work CdS nanoparticles have been successfully synthesized via a hydrothermal method without adding any complex reagent at the 180 °C for 24 h.

### II. EXPERIMENTAL SECTION

#### 2.1 Chemicals

Cadmium nitrate ( $\text{Cd}(\text{NO}_3)_2$ ), sodium sulfide ( $\text{Na}_2\text{S}$ ) and sodium hydroxide (NaOH) chemicals used in this study were of analytical reagent grade purchased from Sigma- Aldrich Pvt. Ltd., Mumbai and used without further purification. Distilled water was used as a solvent.

#### 2.2 Synthesis of CdS nanoparticles

In a hydrothermal synthesis, 0.05M of  $\text{Cd}(\text{NO}_3)_2$  was dissolved in 70ml of distilled water in a beaker. The pH of the solution was maintained at around 11-12 by adding sodium hydroxide (NaOH) under vigorous magnetic stirring to form a clear solution. Then 0.05 M of  $\text{Na}_2\text{S}$  was added to the mixture solution. Then the resultant pale yellow solution was transferred into a Teflon-lined stainless steel autoclave and maintained 180°C for 24h. The resulting powder was washed with ethanol several times and finally dried at 60 °C for 6h. The final yellow powder was then obtained and used for the further characterizations.

#### 2.3 Characterization

The structural study of as-synthesized product was performed using X-ray diffractometer (Rigaku, Miniflex-II) with  $\text{CuK}_\alpha$  ( $\lambda = 1.5406 \text{ \AA}$ ) radiation. The surface morphology and elemental composition analysis were examined by scanning electron microscope (JEOL, JSM-IT300) equipped with an energy-dispersive X-ray spectrometry (EDAX, OXFORD instrument). For optical studies, an optical absorption spectrum was recorded with a Shimadzu UV-1800 spectrophotometer. Photoluminescence study was carried out with a fluorescence spectrophotometer (PerkinElmer LS-55) equipped with a xenon lamp.

### III. RESULTS AND DISCUSSION

#### 3.1 Structural study

The XRD pattern of hydrothermally derived CdS product and relevant information are shown in Fig. 1. The result shows that all peaks are strong and sharp diffraction indicate that the CdS product is well crystallized. The obtained peaks were matching with the reported value of (JCPDS file No. 77-2306) which confirms the hexagonal crystal structure. The strongest peak in the XRD pattern could be indexed to (101) at a  $2\theta$  value of  $28.4^\circ$ . The lattice parameters of hexagonal phase have been calculated by using equation (1) respectively.

$$\frac{1}{d^2_{(hkl)}} = \frac{4}{3} \left( \frac{h^2 + hk + k^2}{a^2} \right) + \frac{l^2}{c^2} \quad (1)$$

Where 'd' is the Interplanar distance and 'h, k, l' are Miller indices of the lattice planes. The lattice parameter 'a' and 'b' of hexagonal phase were found to be in the order of  $4.106 \text{ \AA}$  and  $6.680 \text{ \AA}$  respectively.

The average particle size has been calculated by using scherrer's formula and found to be  $17.06 \text{ nm}$ .

$$D = \frac{K\lambda}{\beta \cos\theta} \quad (2)$$

Where K is constant (0.9),  $\lambda$  is the wavelength of the X-ray used,  $\beta$  is broadening of diffraction line measured at half of its maximum intensity (in rad) and  $\theta$  is Bragg's diffraction angle.

#### 3.2 Compositional study

The EDAX analysis of CdS nanoparticles is shown in Fig. 2. This study exhibits the presence of all elements in the sample i.e. cadmium (Cd) and sulfur (S) and no other impurity elements are observed. From the results it reveals that Cd and S are present in their stoichiometric ratio of Cd: S is 53.04:46.96 which confirms the high purity of synthesized CdS product.

#### 3.3 Morphological study

Figure 3(a-b) shows the SEM images of the CdS nanoparticles by organic -free hydrothermal method at  $180^\circ \text{C}$  for 24 h. The morphology of cluster CdS nanoparticles can be observed from SEM images at different magnification. From SEM images, it is observed that the CdS nanoparticles exhibited spherical granules like structure.

#### 3.4 Optical study

UV-vis absorption spectra of CdS nanoparticles is shown in Fig. 4(a). From UV- vis spectra, it has been observed that the absorption peak is at  $502 \text{ nm}$ . The optical transition between the levels in the conduction and valence bands depends on the size of nanoparticles. The absorption spectroscopy plays an important role in for determination of band gap which can be calculated from Tauc's relation. From Tauc's relation, the absorption coefficient for a direct band gap is given by,

$$\alpha = A (h\nu - E_g)^n / h\nu \quad (3)$$

Where A is constant,  $\alpha$  is the absorption coefficient of semiconductor,  $E_g$  is the band gap,  $h\nu$  is the incident photon energy and n is a constant value, which is equal to  $1/2$  for direct band gap semiconducting materials. The Fig. 4(b) shows the plot of  $(\alpha h\nu)^2$  versus  $(h\nu)$  for CdS nanoparticles. The  $E_g$  of CdS nanoparticles is  $2.47 \text{ eV}$ , which is greater than the standard bulk  $E_g$  value of CdS.

#### 3.5 Photoluminescence study

Figure 5 shows the room temperature PL spectra of CdS nanoparticles under photon excitation of  $390 \text{ nm}$ . There are two emission peaks in the photoluminescence spectrum: one is sharp and narrow peak is located at  $524 \text{ nm}$ , the other is broad and located in the range of  $600\text{-}750 \text{ nm}$ .

#### IV. FIGURES

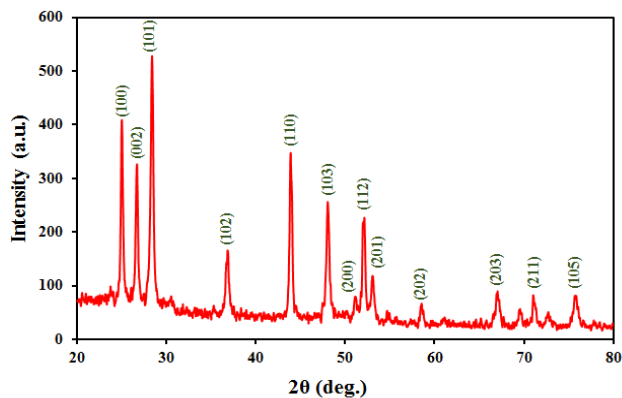


Fig. 1: The XRD Pattern of CdS nanoparticles

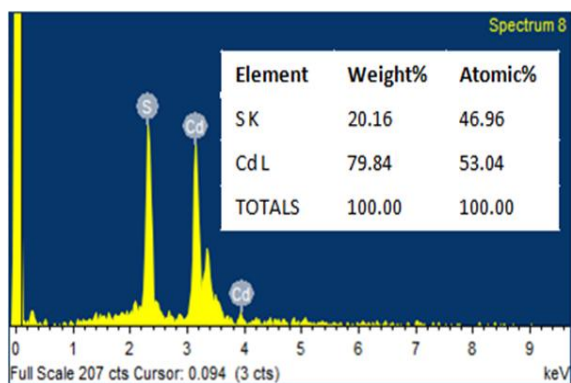


Fig. 2: The EDAX pattern of CdS nanoparticles

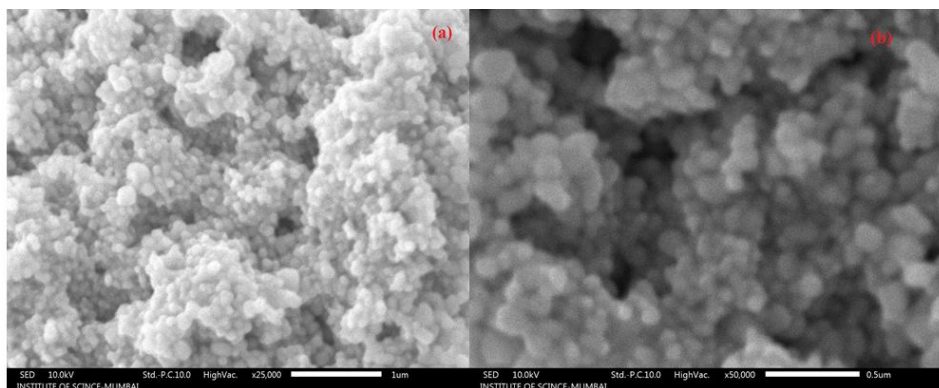


Fig. 3: SEM images of CdS nanoparticles with different magnifications (a) 25 kX (b) 50 kX

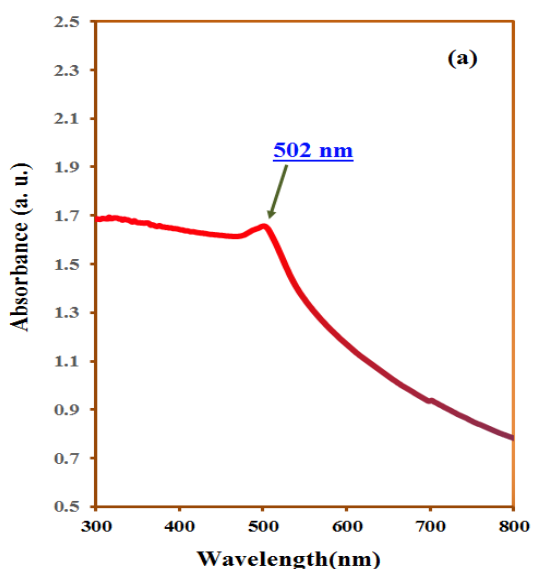


Fig. 4(a): UV-visible absorption spectrum of CdS nanoparticles

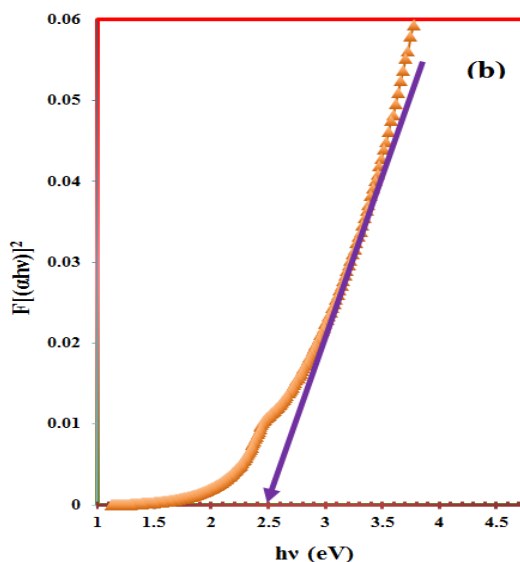


Fig. 4(b): The plot between  $(\alpha h\nu)^2$  and binding energy ( $h\nu$ )

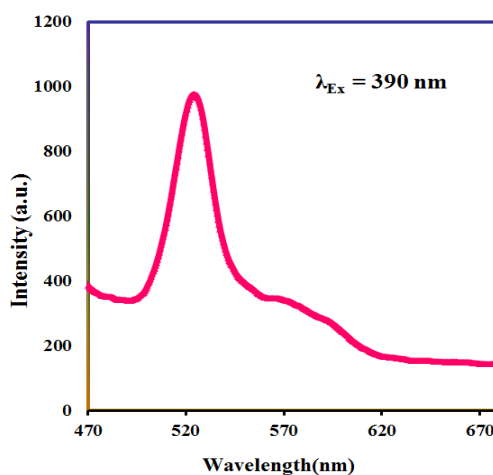


Fig. 5: PL spectrum of CdS nanoparticles

## V. CONCLUSION

The CdS nanoparticles have been successfully synthesized by a simple hydrothermal method without using any capping reagent. XRD study revealed that all the peaks are assigned to the wurtzite structure having a hexagonal phase of the CdS nanoparticles. The compositional analysis study confirmed that the sample is pure CdS. The morphology showed the spherical like structure. The UV- visible study shows the absorption peak at 502 nm and energy band gap was calculated to be 2.47 eV. The PL shows the sharp and narrow emission peak at 524 nm. Depending upon the above properties of the CdS nanoparticles were used in the light emitting diodes, solar cell etc.

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