

# Investigation of Structural and Spectroscopic Properties of Nanostructured CdS Films

P.K. Mochahari

Department of Physics, D.K.D. College, Dergaon, Assam, India  
Corresponding author: mocharip@rediffmail.com, Tel: 9435092953

Available online at: [www.isroset.org](http://www.isroset.org)

Received: 09/Nov/2017, Revised: 17/Nov/2017, Accepted: 14/Dec/2017, Published: 31/Dec/2017

**Abstract-** Nanostructured cadmium sulphide (CdS) films have been prepared on glass substrates by chemical bath deposition (CBD) method at room temperature. Analysis of the samples by x-ray diffraction (XRD) exhibits the films have cubic phase structure of CdS. Different structural parameters such as crystallite size (using Scherrer's relation) and dislocation density of the samples have been estimated. Optical absorption spectra of the sample falls in the visible region and various optical parameters such as optical band gap energy (using Tauc's formula), refractive index as well as dielectric constant have been calculated. Chemical composition of the samples has been investigated using fourier transform infra red (FTIR) spectroscopy.

**Keywords-** XRD, optical band gap, refractive index, FTIR

## I. INTRODUCTION

During recent decade, nanomaterials have attracted great interest and attentions due to their unique characteristics that differ from that of the bulk materials. The novel properties of nanomaterials are size, structure and shape dependent. Semiconductor II-VI nanomaterials have received much importance due to their unique mechanical, optical and magnetic properties as well as applications in various fields. Cadmium sulphide belongs to II-VI group material and it is a special material having direct wide band gap energy (2.42 eV in bulk form) and high refractive index (2.5). It has wide range of applications in numerous areas including multilayer light emitting diode [1], field effect transistor, gas sensor [2], photovoltaic cell [3], optoelectronic devices [4] and many more. Different workers have adopted various techniques to prepare CdS nonmaterials such as sputtering [5], spray pyrolysis [6], electrochemical deposition [7], pulsed laser deposition [8], vacuum deposition [9], chemical deposition, etc. Chemical bath deposition [10] is a simple, widely used, cost effective method which allows large area deposition. In our present paper synthesis of nanostructured CdS films using CBD method and structural, optical as well as spectroscopic investigations are reported.

This paper has been organized into four distinct sections- Introduction, Materials and Methods, Results and discussion and conclusions. In introduction section brief literature review related to our present work is presented. Materials and Method section contain the materials used for the preparation of nanostructured CdS film and details of preparation as well as the characterization instruments used.

Results and discussion section provides XRD spectra, optical absorption spectra, FTIR spectra of nanostructured CdS films and analysis and discussion of the results obtained. In the conclusion section major conclusions drawn from the results are provided.

## II. MATERIALS AND METHODS

### Materials

Monohydrate cadmium chloride ( $\text{CdCl}_2 \cdot \text{H}_2\text{O}$ ) (pure), purchased from Merck specialties private limited, Mumbai, India, nonahydrate sodium sulphide ( $\text{Na}_2\text{S} \cdot 9\text{H}_2\text{O}$ ) (pure), purchased from Rankem, RFCL, New Delhi, India and polyvinyl alcohol (pure) purchased from sd fine CHEM limited, Mumbai, India were used for the preparation of nanostructured CdS films.

### Method

Nanostructured CdS films have been synthesized by ion exchange reaction in the matrix of polyvinyl alcohol (PVA). The matrix solution was prepared by adding  $\text{CdCl}_2$  solution having 1.0 molarity to an aqueous solution (4wt %) of PVA in equal volume under a high stirring rate 200 rpm for 3 hours at constant temperature  $70^\circ\text{C}$ . The prepared solution was kept for 12 hours for complete dissolution. Next,  $\text{Na}_2\text{S}$  solution having 0.25 molarity was added to the above solution till the whole solution turns into yellow colour and stirred for 15 minute. The final CdS solution was casted on cleaned glass substrates and are allowed to dry in a closed chamber at room temperature to yield nanostructured CdS films.

### Characterization

Structural characterization of prepared nanostructured CdS film was done by XRD using Bruker (AXS D8 Advance) with  $\text{CuK}\alpha$  radiation ( $\lambda=1.5406\text{\AA}$ ). CARY 300 Scan UV-Visible spectrophotometer was used to record optical absorption spectra in the wavelength range 350nm-800nm at room temperature. Fourier transform infra red (FTIR) spectra of nanostructured CdS film was recorded in IR Affinity-1, SHIMADZU in the wavelength range of 4000 to 450  $\text{cm}^{-1}$ .

## III. RESULTS AND DISCUSSION

### X-Ray Diffraction (XRD) study

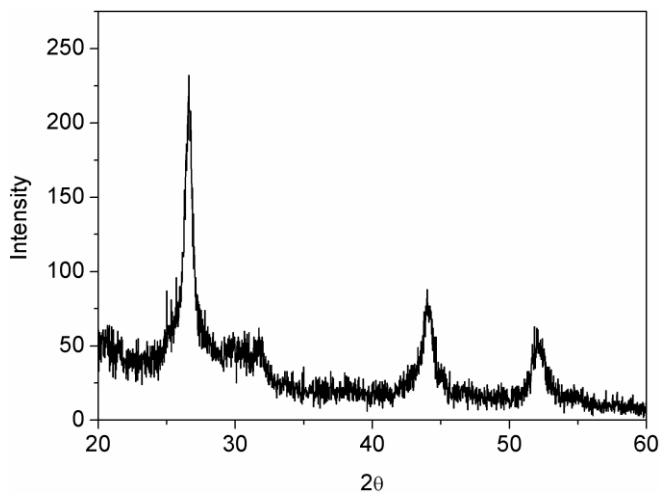


Fig 1: XRD pattern of nanostructured CdS film

XRD pattern of prepared nanostructured CdS film (1.0 molarity) is shown in Fig. 1. The XRD pattern exhibits three prominent and clear peaks centered at  $2\theta=26.73$ ,  $44.23$ ,  $52.41$  which can be assigned to (111), (220) and (311) planes respectively of the CdS cubic crystalline phase (JCPDS-800019). The peak position of (111) plane is found to shift towards higher diffraction angles by  $0.183$  compared to its corresponding value for bulk CdS ( $2\theta=26.547$ ; JCPDS - 800019) indicating formation of compressive stress. The formation of compressive stress may be attributed to residual stress generated in the film during deposition or due to the lattice mismatch between the film and the substrate [11]. The formation of intense and broad diffraction peak profile indicates generation of good nanocrystal. The interplanar spacing ( $d$ ) is estimated from Bragg's equation ( $\lambda=2d\sin\theta$ ).

The calculated value of lattice constant ( $a$ ) is found from the relation  $a = d(h^2 + k^2 + l^2)^{1/2}$ . The values of both interplanar spacing ( $d$ ) and lattice constants are cited in Table 1. The crystallite size ( $D$ ) of the prepared sample is estimated using Scherrer's formula [12].

$$D = \frac{K\lambda}{\beta \cos \theta} \quad (1)$$

Where  $K$  is a constant equal to  $0.94$ ,  $\lambda$  is the wavelength of the radiation which is  $1.54056 \text{\AA}$  for  $\text{CuK}\alpha$  radiation,  $\beta$  (in radian) is the full width at half maximum (FWHM) of the peaks and  $\theta$  is the Bragg's diffraction angle. The calculated value of crystallite size is cited in Table 1.

Dislocation density of nanostructured CdS film has been estimated using the relation [13]

$$\text{Dislocation density } (\delta) = 1/D^2 \quad (2)$$

Where  $D$  is the crystallite size. The estimated value of dislocation density of the sample is cited in Table 1.

**Table 1** Structural parameters of nanostructured CdS film

Sample	$2\theta$ (degree)	$d$ value ( $\text{\AA}$ )	( $hkl$ )	$a$ ( $\text{\AA}$ )	Crystallite size $D$ (nm)	Dislocation density ( $\delta$ ) $\times 10^{16}/\text{m}^2$
CdS (1.0 M)	26.73	3.332	(111)	5.772	9.5813	1.0595
	44.23	2.046	(220)	5.787		
	52.41	1.744	(311)	5.785		

### Optical absorption study

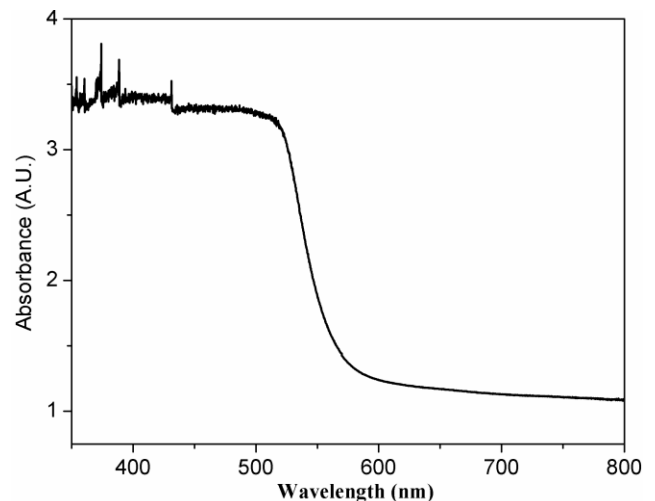


Fig 2: Absorption spectra of nanostructured CdS film

The knowledge of optical absorbance and band gap energy is important for material to be used in the solar cell fabrication. Fig. 2 shows optical absorbance curve in the range 350- 800 nm for 1.0 molarity nanostructured CdS film deposited at room temperature. Optical absorption spectra of the sample shows sharp absorption edge in the visible region which

indicates good crystallinity as well as low defect density near band edge [14].

The optical band gap energy ( $E_g$ ) is estimated using Tauc's formula [15]

$$(\alpha h\nu)^{1/n} = A(h\nu - E_g) \tag{3}$$

Where  $\alpha$  is the absorption co-efficient,  $h\nu$  is incident photon energy,  $A$  is a constant. Since CdS is a direct band gap material, so,  $n=1/2$  for allowed transition. Band gap energy has been found by extrapolating the linear region of the plots  $(\alpha h\nu)^2$  versus  $h\nu$  on the energy axis as shown in Fig. 3. The band gap energy is found to be 2.56 eV (cited in Table2) which is blue shifted compared to the value of bulk CdS and it is attributed to size (quantum confinement) effect [16].

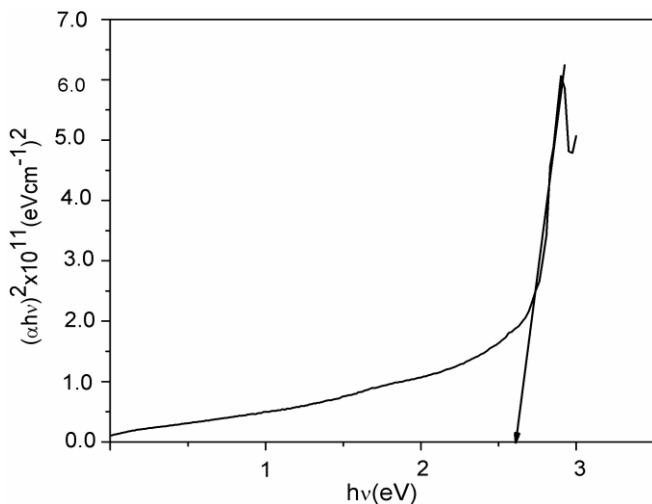


Fig 3:  $(\alpha h\nu)^2$  vs  $h\nu$  plot of nanostructured CdS film for band gap determination

Refractive index for the prepared sample is determined from the relation given by Herve and Vandamme [17]

$$n = \sqrt{1 + \left(\frac{A}{E_g + B}\right)^2} \tag{4}$$

Where  $A=13.6$  eV and  $B=3.4$  eV are constants. This relation is accurate for the materials having high band gap. The estimated value of refractive index for the sample is cited in Table 2.

Optical dielectric constant ( $\epsilon_a$ ) is calculated from the relation [18]

$$\epsilon_a = n^2 \tag{5}$$

Where  $n$  is the refractive index. The estimated value of dielectric constant for the sample is cited in Table 2.

**Table 2** Optical parameters of nanostructured CdS film

Sample	Band gap energy, $E_g$ (eV)	Refractive index	Dielectric constant ( $\epsilon_a$ )
CdS ((1.0 M)	2.56	2.49	6.20

**Fourier Transform Infrared (FTIR) study**

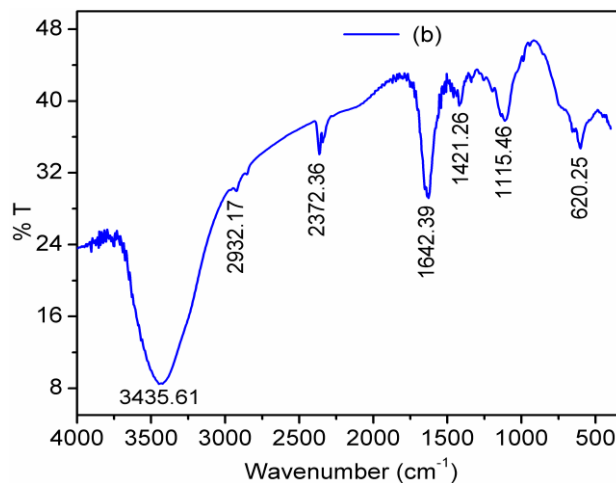


Fig 4: FTIR spectra of nanostructured CdS film

FTIR spectroscopy is an important technique to determine the functional group. It is a useful method to find bond vibration frequency in a molecule. FTIR spectra of nanostructured CdS sample prepared in PVA matrix at room temperature is shown in Fig. 4. The absorption band at  $3435.61\text{ cm}^{-1}$  is attributed to the O-H stretching vibration of water molecule [19]. The band at  $2932.17\text{ cm}^{-1}$  is due to C-H stretching. The absorption band which appears at  $1642.39\text{ cm}^{-1}$  is assigned to C=O stretching. The absorption band at  $1421.26\text{ cm}^{-1}$  is due to C-H stretching. Trace amount of  $\text{SO}_4^-$  is observed with the appearance of absorption band at  $1115.46\text{ cm}^{-1}$  [20]. The medium band at  $620.25\text{ cm}^{-1}$  has been assigned to Cd-S stretching [21].

**IV. CONCLUSION AND FUTURE SCOPE**

Good quality nanostructured CdS films have been successfully synthesized on glass substrates by chemical bath deposition method. Structural study using XRD method shows the formation of cubic phase structure and crystallite size of the sample is found to be  $9.5813\text{ nm}$  whereas dislocation density is  $1.0595 \times 10^{16}/\text{m}^2$ . The band gap energy of the sample estimated to be  $2.56\text{ eV}$  is blue shifted compared to the value of bulk CdS due to quantum confinement effect. Refractive index and dielectric constant are found to be  $2.49$  and  $6.20$  respectively. Investigation of FTIR spectra shows the stretching modes of the sample. We plan to study electrical and magnetic properties of the nanostructured CdS films as our future work.

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## AUTHOR PROFILE

Dr. Prince Kumar Mochahari pursued BSc. from St. Anthony's College, Shillong. He did MSc. in Physics from NEHU, Shillong. He obtained PhD degree from Gauhati University in the year 2016. His area of study during PhD research work is Thin Film Nano and ion implantation in the sample materials. He is currently working as Asstt. Professor in the department of Physics, D.K.D.College, Dergaon, Assam, India. He has published good number of research papers in reputed international journals including SCI. Moreover he has presented large number of research papers in international and national conferences/seminars.

