

*Research Paper*

## **Structural Properties of CdS Nanoparticles for Solar Cell Applications**

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**Abstract:** *The cadmium sulphide (CdS) is an important II–VI semiconductor ( $E_g = 2.42$  eV, 515 nm) at room temperature with many excellent physical and chemical properties. It has promising applications in multiple technical fields including photochemical catalysis, gas sensor, detectors for laser and infrared, solar cells, nonlinear optical materials, various luminescence devices, optoelectronic devices etc. CdS being a wide band gap semiconducting material with better lattice matching properties made it suitable alternative for solar cell applications. Solar energy is the alternative potential renewable energy to fossil fuels. Present work deals with a co-precipitation synthesis method for the preparation of CdS nano particles. In this method cadmium sulphate and thiourea are used as a source material for Cd and S respectively in the presence of N, N-Dimethyl formamide (DMF) as an organic solvent. The CdS nano particles have been characterized by X-Ray Diffraction (XRD), Particle Size Analyzer (PSA), Scanning Electron Microscope (SEM), Energy Dispersive X-ray Spectrometry (EDX).*

**Keywords:** CdS nanoparticles, Co-precipitation method, XRD, SEM, Solar Cell.

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### **1. Introduction:**

CdS (Cadmium Sulphide) particles are II – VI semiconductor materials with the band gap 2.42 eV. They show very good physical and chemical properties thus the nano crystalline semiconductor materials having wide range band gaps. [1, 2]. The physical and chemical properties shown by these

nano range particles are due to their crystallite size. Additional growth of the crystallite size is from bulk particles [3]. CdS is an important semiconductor photocatalyzer. In order to explore more suitable applications or acquire the enhanced properties, different morphological CdS nanomaterials have been synthesized by sputtering, vapour-phase condensation, sol-gel reaction, micro emulsion reaction, template-assisted reaction, chemical hydrolytic reaction, etc [4, 5]. The nanometer range semiconductors have applications in various fields like solar energy conversion, opto electronic industry and photo catalysis [6].

The present work deals on the synthesis of CdS nanoparticles by Co-precipitation synthesis method. CdS nanoparticles are characterized by using XRD and PSA for the study of average crystallite size, SEM for morphology studies, EDX for compositions of the elements respectively.

## 2. Experimental Details:

Co-precipitation synthesis method is very simple, fast, cost and time efficient. It gives less nano range particles compared with other techniques like hydrolysis method, sol-gel synthesis, template-assisted reaction, microwave-solvo thermal method etc. CdS nanoparticles are synthesized by a novel co-precipitation synthesis with starting materials cadmium sulphate and thiourea in presence of organic solvent DMF without any capping agent. The pH was maintained 9 using NaOH solution added drop-wise with vigorous stirring. The transparent solution turns into light yellow color and after completion of reaction it turns in dark yellow. The precipitate then washed several times with ethanol and water. The precipitate is further dried at 800C for 30 minutes which leads to the formation of CdS nanoparticles.

## 3. Results and Discussion:

The XRD pattern of the CdS nano particles obtained from co-precipitation synthesis are as shown in Fig 1. The result showed that the structure of the CdS nano particles was in hexagonal phase. The peaks broadening represented the dimensions of the nano range particles. Peaks were observed at  $28.183^\circ$ ,  $43.682^\circ$  and  $54.586^\circ$  respectively which corresponded to (1 0 1), (1 1 0) and (0 0 4) planes respectively.

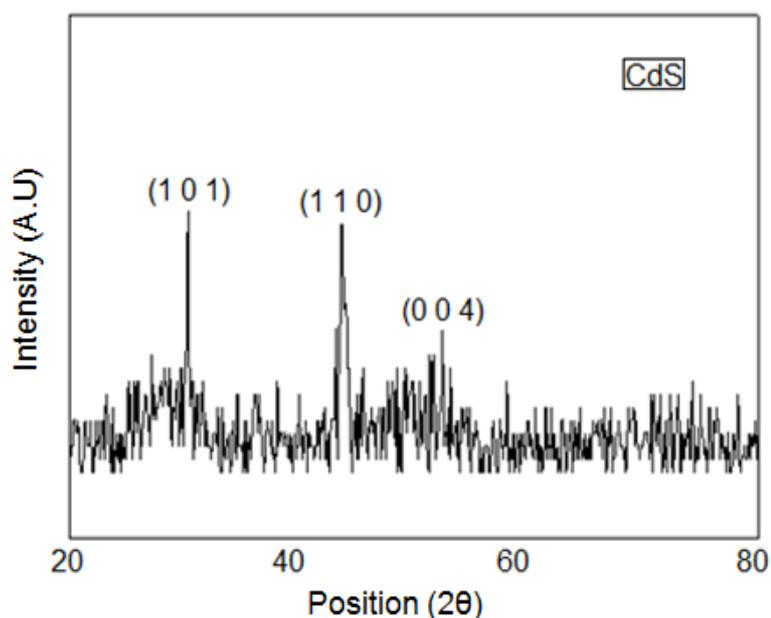


Fig. 1: XRD pattern of CdS nanoparticles

The lattice parameters were in good agreement with JCPDS card number 41 – 1049 having lattice parameters  $a = b = 4.140 \text{ \AA}$ ,  $c = 6.719 \text{ \AA}$ . The crystallite size was calculated using Debye – Scherrer's formula, we observed the average crystallite size as 35 nm.

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

where  $D$  is the average crystallite size of the particle,  $\lambda$  is the wavelength of the radiation,  $\beta$  is the full width half maximum (FWHM) of the peak,  $\theta$  is the Bragg's angle.

The strain and crystallite size of the sample were measured from the Williamson Hall equation

$$\beta \cos \theta = \frac{\kappa \lambda}{t} + 2\epsilon \sin \theta \quad (2)$$

where  $\beta$  is the full width half maximum (FWHM) of the XRD corresponding peaks,  $k$  is Debye-Scherer's constant,  $t$  is the crystallite size,  $\lambda$  is the wave length of the X-ray radiation,  $\epsilon$  is the lattice strain and  $\theta$  is the Bragg angle. In this process  $2\sin\theta$  is plotted against  $\beta\cos\theta$ , using a linear extrapolation to the plot, the intercept gives the crystallite size and slope gives the strain ( $\epsilon$ ). The crystallite size measured as 25 nm and the strain obtained as  $5.86 \times 10^{-3}$ .

The lattice parameters of the hexagonal phase were measured using the formula

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

The measured values  $a = b = 0.40819 \text{ nm}$  and  $c = 0.67196 \text{ nm}$  were shows the similar values which is from the XRD pattern.

The as-prepared CdS nanoparticles were ultra-sonicated and suspended in the ethanol solution. The histograms of the particle sizes vs undersize percentages were shown in Fig 2. The CdS nanoparticles were analysed by the dynamic light scattering which showed the mean particle size as 39 nm. It corresponds with the crystallite size (35 nm) calculated from the XRD pattern.

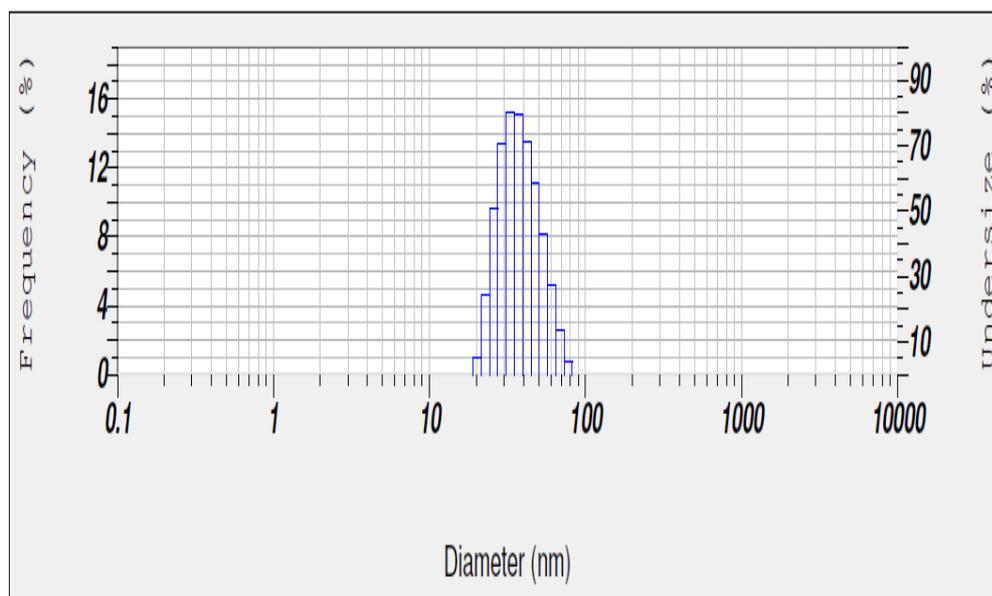
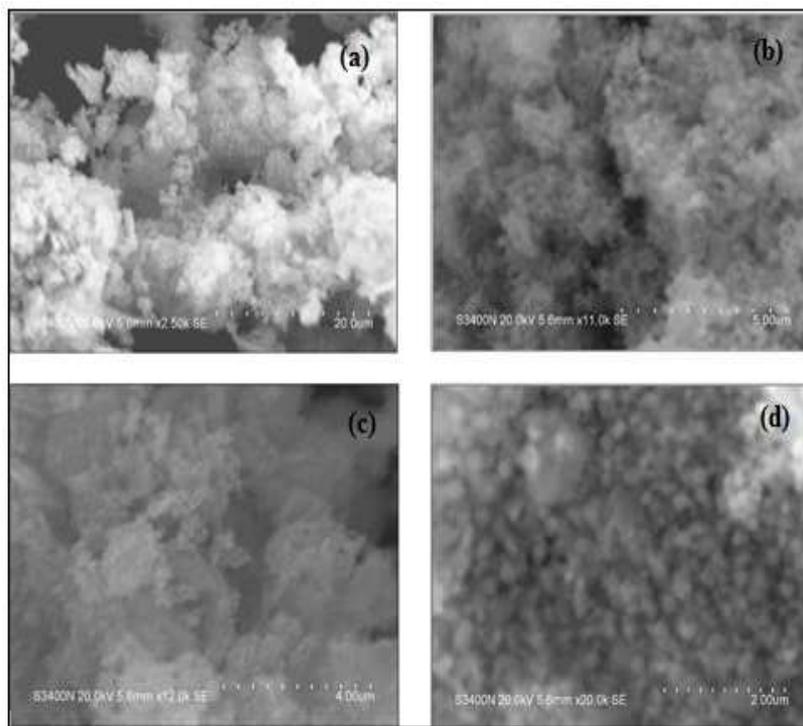


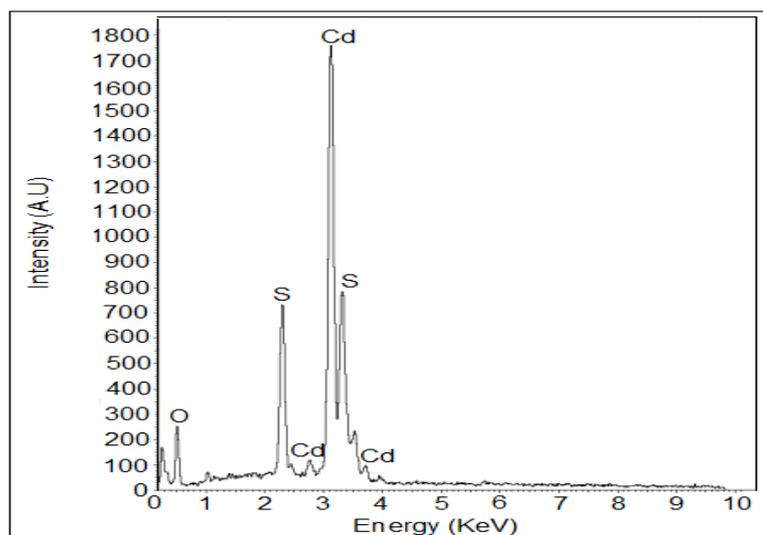
Fig. 2: Particle distribution of CdS nanoparticles

The grain size, shape and surface morphology were observed by the SEM with different magnifications as shown in Fig 3. It showed that the particles exhibited spherical granules like structure [7].



**Fig. 3:** SEM images of the CdS nanoparticles

The elemental percentages obtained from EDX pattern of Cadmium, Sulphur and Oxygen are 60.04%, 32.18% and 7.78% respectively. EDX pattern of as-synthesized sample is as shown in Fig 4. It showed that the nano particles having the different compositions of Cadmium and Sulphur [8].



**Fig. 4:** EDX spectrum of CdS nanoparticles

#### 4. Conclusions:

The CdS nanoparticles were successfully synthesized using the precursor materials cadmium sulphate as the source of Cd<sup>2+</sup> ions and thiourea as the source of the S<sup>2-</sup> ions by the co-precipitation synthesis. The XRD results indicated the presence of hexagonal phase in the sample and the crystallite size 35 nm was calculated with Debye-Scherrer's formula. Particle size histogram showed the particle size as 39 nm. The SEM images showed spherical granules like structure. EDX pattern inferred, the presence of elements Cd, S and O. Depends upon the above properties these nano sized particles are used in solar cell applications.

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