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Studies on Cobalt Doped CdS Nanoparticles by Simple Co-Precipitation Route

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Abstract: This study examined the influence of the Co doping concentration on the structural and optical properties of $Cd_{1-x}Co_xS$ nanoparticles synthesized using simple Co-precipitation route at room temperature. The samples were characterized by X-ray diffraction and FTIR spectroscopy. From XRD patterns, Co doped CdS nanoparticles have cubic crystal structure with single in phase. The lattice constant and volume of unit cell were increased with increasing Co doping. The crystallite size of prepared nanoparticles increased with increasing Co content from 2.07 to 2.57 nm. The pure and Co doped CdS samples have spherical like structured. The dislocation density and strain was decreased with increasing Co doping. The functional groups of the nanoparticles have been identified by FTIR studies. The results showed that Co doping strongly affects the structural and optical properties CdS nanoparticles.

Keywords: Nanocrystals; CdS; dislocation density; strain; FTIR study.

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I. INTRODUCTION

Nanoparticles are in hunge expansion worldwide due to its unique functional properties. A great effect has been made to the design and controls the development of nanoparticles such as CdS. CdS is an efficient window material that belongs to the II-IV group semi-conducting material with wide band gap energy of 2.4 eV. CdS are one of the most promising materials for optoelectronic device such as lasers, gas sensors, detectors, optoelectronics devices, light emitting diodes and solar cells [1-4]. Wide band gap of CdS has been used as good photoconduction, high electron affinity and inexpensive synthesized route [5-7]. CdS is n-type semiconductor used as the window materials for hetro-junction in solar cells usually has a high absorption coefficient causing the reduction of the useful current delivered from the cell to the load [8].

The synthesis of CdS materials has been explored by different techniques such as electrochemical synthesis [9], chemical bath deposition [10], thermal evaporation [11], chemical vapor deposition [12], pulse laser deposition [13], spray pyrolysis [14] etc. The route of CdS also significant impact on the particle size which is important role in photocatalytic applications, room temperature LPG gas sensor [15-16]. The reported methods are expensive and requires sophistication as compared to co-precipitation route, so we have choose this techniques due to its simplicity low-cost and availability of the equipments. Crystal phase and average crystallite size were measured using XRD. SEM is used to study the particle size and morphology. Functional groups of Co doped CdS nanopartcles were study using FTIR.

II. EXPERIMENTAL DETAILS

$Cd_{1-x}Co_xS$ samples for concentration x = 0.00, 0.01, and 0.02 are prepared by co-precipitation route. Appropriate amount of analytical grade of Cadmium acetate dehydrate and sodium sulfide dissolved in separate beaker of distilled water and under vigorous stirring for 2 h to obtain homogeneous and clear solution. Drop by drop added the sodium sulphide to obtain ppt (PH 13.5). A white precipitate was obtained which was separated by centrifugation. The precipitate which is separated is washed several times with distilled water and ethanol then dried under vacuum at 60 ^oC to get the powder samples of CdS nanoparticles. For the synthesis of Co doped CdS nanoparticles were prepared at room temperature by mixing calculated amounts of Cadmium acetate solution and Cobalt acetate solution followed by drop wise addition of saturated solution of sodium sulfide up to pH 13.5. The mixture was vigorously stirred for 2 h. The precipitate was filtered from the reaction mixture and washed several times with ethanol to remove all sodium particles. The wet precipitate was then dried. Similarly prepared for samples of 1%, 2% Co doped CdS samples.

Structural characterization of prepared samples was measurement using x-ray diffraction (Model: PW-3710). The structural analysis of the synthesized samples was carried out using a powder X-ray diffractometer (XPERT-PRO) with a Cu-Kα radiation source of wavelength 1.5406 A^0. The crystalline structure, phase purity and size of the nanoparticles were determined by X-ray diffraction (XRD) using X-ray diffractometer (Model:

PW-3710) employing Cukα radiation. Fourier Transform Infrared (FTIR) spectra of all samples recorded using JASCO FI-IR 460 spectrometer in the range 400-4000 cm^{-1} by KBr pellet technique.

III. RESULTS AND DISCUSSION

Figure 1 present XRD patterns of the Co:CdS nanoparticles with different molar ratio of Cobalt. The XRD peaks were clearly indexed to the cubic signal phase [17] with lattice constant a= 5.3763 Å. The XRD peaks at 28.66°, 48.19° and 56.43° were assigned to the (111), (220) and (311) reflections of CdS phase respectively. No XRD peaks of Cobalt were observed, which indicated that Co had entered the CdS host lattice matrix. The intensities of the major peaks at (111) and (220) increases with increasing Co doping content. The CdS (111) and (220) peak position shifted to lower angles for the doped CdS samples as compared to pure CdS nanoparticles, indicating contraction of the CdS lattice due to the substitutions of Co ions into the Cd ions. Generally, if Co ions doping for Cd then lattice should contact because the ionic radius of Co ions and Cd ions was respectively.

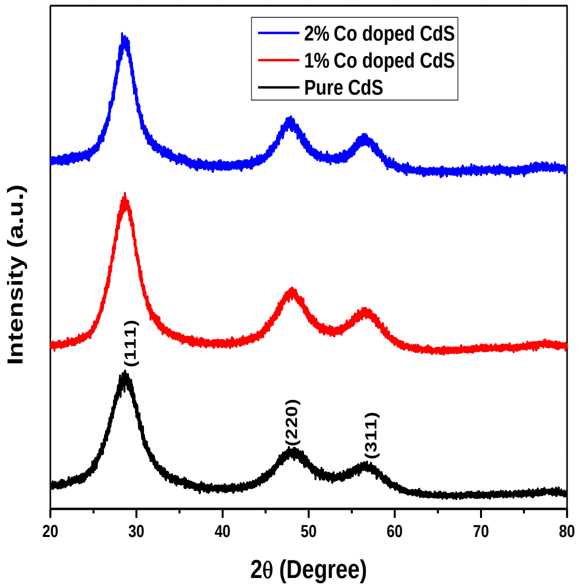

Figure 1. XRD patterns of pure and Co doped CdS nanoparticles.

The lattice constant of nanoparticles were calculated from XRD data and given in table 1. From table 1, it was observed that the lattice constant increased with increasing Co doping content. In addition, the volume of unit cell increases with increasing Co doping concentration, due to the enhancement of lattice constant.
The average crystallite size was calculated using Scherrer's equation is given by

$$D = \frac{0.9\lambda}{\beta \cos\theta}$$

Here, D is crystallite size, λ is the X-ray wavelength (Cu Kα; 1.5405 Å), β is full width at half maximum (FWHM) in radians, θ is the Bragg´s angle in degrees, K is the correction factor and D is the crystallite size. The average crystallite size increased with increasing Co content and is in the range of 2 to 3 nm. It may be due to the small grain growth of CdS nanoparticles as compared to the Co doped CdS nanoparticles. Giribabu et al. [18] reported that pure and Co-doped CdS nanoparticles size around 3 nm. The strain was determined using formula:

The strain reduced with increasing Co doping in the CdS host lattice matrix. This attributed due to the increasing the average crystallite when Co increased. The dislocation density was estimated using crystallite size. The values of dislocation density were decreased with increasing Co content. The strain and dislocation density depends upon the average crystallite size. The strain and dislocation density is tabulated in table 1.

$$\varepsilon = \frac{\beta}{4\tan\theta}$$

Table 1: Lattice constant, volume, crystallite size, strain and dislocation density of Co doped CdS nanoparticles.

Samples	Lattice Constant (Å)	Volume (Å)^3	Crystallite size (nm)	Strain	Dislocation density
Pure CdS	5.3763	155.40	2.07	0.0484	2.32E+17
1% Co	5.3816	155.86	2.25	0.0438	1.96E+17
2% Co	5.3886	156.47	2.57	0.0388	1.50E+17

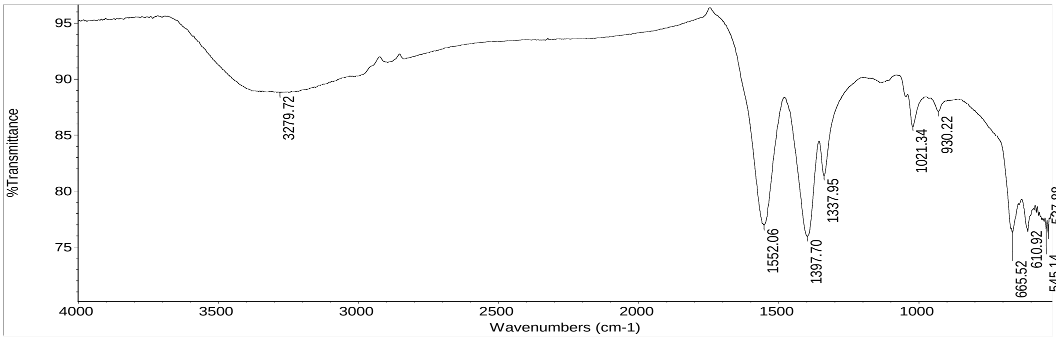

Figure 2(a). FTIR spectra of pure CdS nanoparticles.

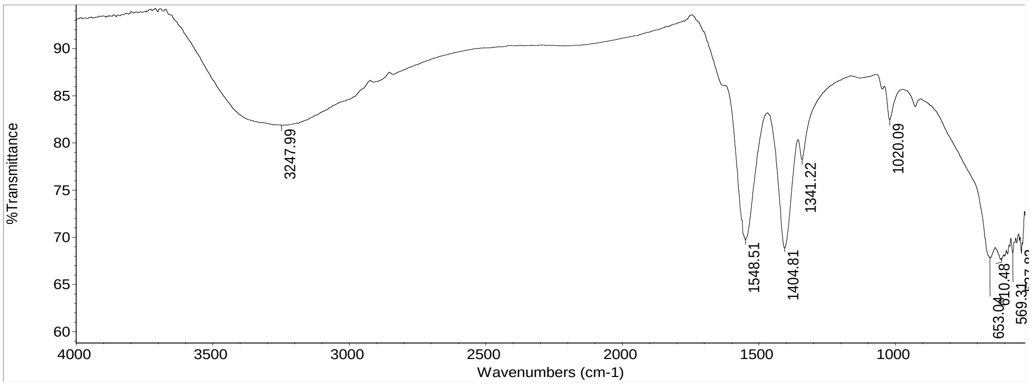

Figure 2(b). FTIR spectra of 1% Co doped CdS nanoparticles.

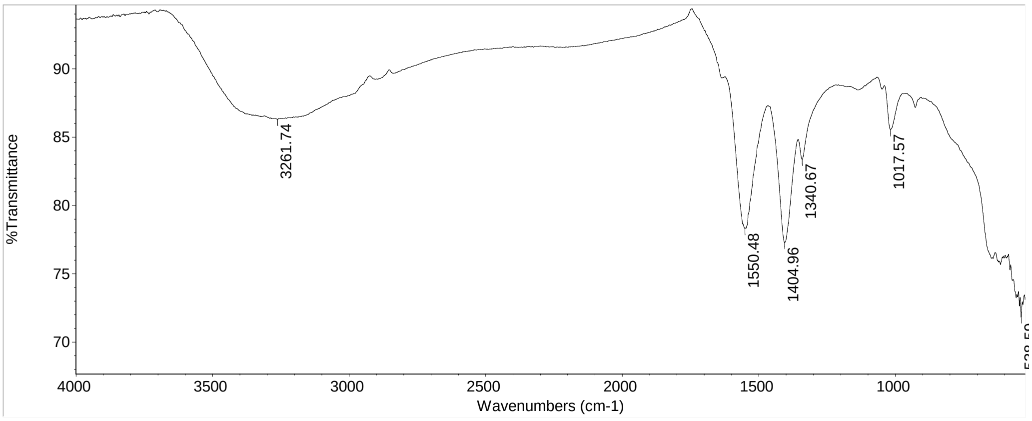

Figure 2(c). FTIR spectra of 2% Co doped CdS nanoparticles.

Figure represents the FTIR spectra of pure and Co doped CdS nanoparticles in the range 400-4000 cm^{-1}. The peak values of FTIR spectra for all grown samples are observed at room temperature and are listed in table 2. The broad peak at 3400 - 3600 cm^{-1} is due to OH stretching vibrations of water molecules indicating the existence of water absorbed on nanoparticles surface. The peak in the range 1400-1757 cm^{-1} is due to OH bending of adsorbed moisture in the sample and all the other peaks are attributed to the characteristic of the material. The bands appeared near at 2000-2200 cm^{-1} indicates the CO adsorption on the surface of oxide. The Cd-S stretching mode Cd^{+2} weak interactions observed in the range of 600-700 cm^{-1}. The FTIR spectrum of the absorption band is due to Co-S stretching of CdCoS in the range of 600 – 400 cm^{-1}. FTIR spectra of pure sample of the present investigation are similar to that of 2% doped CdS samples and are in good agreement with the reported values [19-21].

IV. CONCLUSIONS

Cobalt doped Cadmium sulphide cubic phase nanoparticles were synthesized by co-precipitation chemical route method. The XRD and FTIR spectra indicate that the Cobalt was doped into the crystal lattice and enhances the crystallinity. The lattice constant and volume of unit cell increases with increasing Co doping concentration. The size of nanoparticles was found by XRD to increase with increasing concentration of Co. The values of the strain decreased with increasing Co content due to the increasing crystallite size. The FTIR spectrum of the main absorption band is due to CdMn-S stretching of CdS in the range of 700 – 400 cm^{-1}. Further, FTIR study also shows functional groups Co-S in CdCoS nanoparticles and changing in the wave number with Co doping content.

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