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Research Article

**STUDY OF OPTICAL AND THERMAL PROPERTIES OF  
CHEMICALLY SYNTHESIZED CDS NANOPARTICLES****R. P. Pawar**Department of Chemistry, Government Vidarbha Institute of Science and Humanities Amravati,  
Maharashtra 444604 Email: ramkrupawar@gmail.com**Abstract:**

*Different samples of Cds nanoparticles were synthesized by Wet Chemical rout method at room temperature using cadmium acetate as cadmium source and sodium sulphide as sulphur source. Structural properties of synthesized Cds nanoparticles were performed by X-ray diffraction pattern (XRD) while optical properties were examined by UV-Visible absorption spectroscopy. XRD pattern showed the as synthesized Cds nanoparticles have cubic zinc blende structure with 2.0-2.87 nm average crystallite size and lattice constant  $a=5.829 \text{ \AA}$ . UV-Visible absorption spectrum showed the band gap energy of the Cds nanoparticles corresponding to absorption edge are found in the range of 2.63eV-3.87eV, which shows increase in band gap with the decrease of crystallite size of the nanoparticles.*

**Key Words:** Cds nanoparticles, XRD, UV-Vis spectrum, TGA, Band gap.**\*Corresponding Author:****R. P. Pawar,**

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**INTRODUCTION:**

Nanoparticles having typical dimensions of 1-10 nm have attracted great interest in the past decade as well as in recent years because of their unique chemical, physical, electronic, optical and transport properties which are drastically different from those of either the bulk materials or single atoms.<sup>1,2</sup> Since novel properties of nanomaterials depend on their size, structure and shape,

a new direction for synthetic methods and an understanding of the mechanisms by which the size, structure and shape of the nanocrystals can be easily varied are key issues in nanoscience<sup>3</sup>. Binary chalcogenide nanocrystalline semiconductors such as Cds, Cdse, CdSe and CdS attracted considerable attention in recent years due to their unique properties, which arise due to size quantization. Among them, cadmium sulfide (Cds) is one of the most important group II–VI semiconductor having a typical band gap ( $E_g = 3.42$  eV(515 nm) at room temperature with many excellent physical and chemical properties, which 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, biological labels, waveguides, and photoconductors etc<sup>4-9</sup>. Cds can be obtained in thin film form, or in powder by using different solvents such as water, methanol, dimethyl formamide, dimethyl sulphoxide etc<sup>10,11</sup>. In last decades, efforts have been devoted to the preparation of high - quality Cds nanoparticals and the investigation of optical properties<sup>12</sup>. In present work, Cds nanoparticles were prepared by Wet Chemical rout method without using capping agent. Structural properties have been studied by X-raydiffraction and the energy band gap values were calculated by using the UV-visible spectrophotometry.

**MATERIAL AND METHODS:**

All the chemicals were purchased from analytical grade and used without further purification. Double distilled water was used as a solvent in all the experiments. In the present work, different sized Cds nanoparticles have been prepared by Wet Chemical rout method at room temperature<sup>13</sup>. Cds nanoparticles have been prepared with different molar concentration using cadmium acetate  $Cd(CH_3COO)_2 \cdot 2H_2O$  and sodium sulphide ( $Na_2S \cdot 7H_2O$ ) as source materials without using capping ligand. For synthesis, the cadmium acetate and sodium sulphide were taken in different molar concentration. cadmium acetate (1.0M) and sodium sulphide (1.0M) were dissolved in 100 ml double distilled water separately and so obtained molar solution were stirred

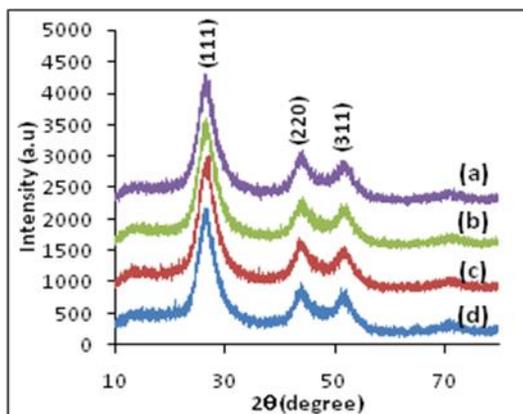
continuously separate for 20 minutes .While stirring cadmium acetate, freshly prepared sodium sulphide 1.0M solution of 100 ml was mixed drop by drop in 100 ml and 1.0 M solution of cadmium acetate. The yellow precipitates of the Cds nanoparticles were formed slowly in the solution. The obtained precipitate was then filtered washed and dried at room temperature. After sufficient drying, the precipitate was crushed to fine powder with the help of mortar and pestle. Four different samples Cds-I ,Cds-II, Cds-III and Cds-IV were prepared by changing the molar concentration as 0.4M, 0.6M, 0.8M, 1.0M.

**FINDINGS:****Structural properties**

X-ray powder diffractions (XRD) were performed at room temperature on a Miniplex-ii X-ray diffractometer using monochromatic  $Cu K_{\alpha 1}$  radiation with  $\lambda=1.540562$  Å° operated at 40 kV and 40 mA with  $2\theta$  ranging from  $10^\circ$  to  $80^\circ$  at the speed of  $2^\circ$   $min^{-1}$ . The diffraction pattern obtained of Cds nanoparticles were prepared with different molar concentration of parent solution. Different sizes of nanoparticles have been prepared by changing the molar concentration of the parent samples as 0.4 M, 0.6 M, 0.8 M and 1.0 M of Cds-I , Cds-II, Cds-III and Cds-IV, respectively. From Fig.(1), XRD patterns obtained in all samples shows three peaks, which shows that the samples have cubic zinc blende structure and the peaks correspond to diffraction at (111), (220) and (311) planes respectively. The lattice parameter has been computed as 5.82 Å°, which is very close to the standard value (5.83 (Å°)). It is also seen that peaks are broadened for higher concentration of parent solution of Cds sample. The peak broadening at lower angle is more meaningful for the calculation of particle size, therefore size of nanocrystals has been calculated using Debye-Scherrer formula<sup>14</sup> given as

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

Where D is the crystallite size, K is constant,  $\lambda$  is the wavelength of x-rays,  $\beta$  is the full width at half maximum (FWHM) after correcting the instrument peak broadening ( $\beta$  expressed in radians),  $\theta$  is the Bragg's angle.



**Fig. 1: XRD patterns of Cds nanoparticles.**  
(a) Cds-I (b) Cds-II (c) Cds-III (d) Cds-IV

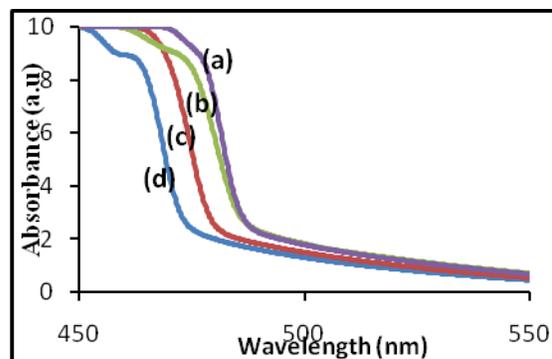
### Optical Absorption :

UV-Visible absorption spectroscopy is an efficient technique to monitor the optical properties of quantum sized particles. The optical absorption spectra of the nanocrystallinities were measured using double beam automated UV-Vis spectrophotometer, and absorption spectra have been recorded at room temperature over the range 450 to 550 nm. The most dramatic property of semiconductor nanocrystals were determined, the band gap energy from the optical absorption spectra. The study of optical absorption is important to understand the behavior of semiconductor nanocrystals. A fundamental property of semiconductors is the band gap, the energy separation between the filled valence band and the empty conduction band. Optical excitation of electrons across the band gap is strongly allowed, producing an abrupt increase in absorption at the wavelength corresponding to the band gap energy. This feature in the optical spectrum is known as the optical absorption edge. Fig (2) shows the optical absorption spectra of Cds nanoparticales in the range of 450 to 550 nm . It can be seen that the absorption occurs in visible region, at 486 nm, 484nm, 478nm, 471nm, for Cds-I , Cds-II, Cds-III and Cds-IV samples respectively. This clearly shows that the absorption edge shifts towards shorter wavelength as the molar concentration is increases. The observed blue shift in the absorption edge is reflection of band gap increase owing to quantum confinement effect.

The energy band gap of material is calculated using the Tauc relation<sup>15</sup>. The relation between the absorption coefficient ( $\alpha$ ) and the incident photon energy ( $h\nu$ ) can be written as  $(\alpha h\nu) = A (h\nu - E_g)^n$

Where, A is a constant,  $E_g$  is the band gap of the material and exponent n depend on the type of transition. Here, the transition are direct so we take

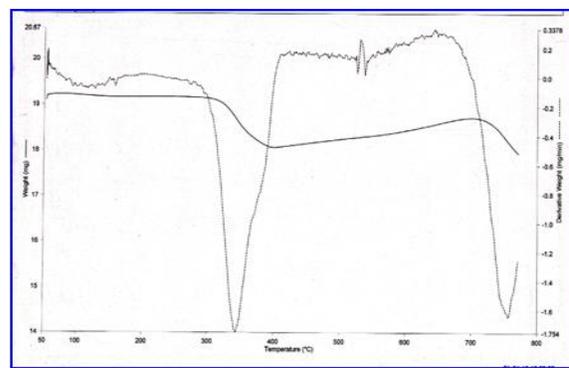
$n=1/2$ . The value of optical band gap is calculated by extrapolating the straight line portion of  $(\alpha h\nu)^2$  vs  $h\nu$  graph (fig. 3.) to  $h\nu$  axis at  $\alpha=0$ . The obtained band gap values for different samples are 2.63, 2.79, 2.81, 2.87 eV respectively.



**Fig .2: Absorption spectra of different samples of Cds nanoparticles.**  
(a)Cds-I (0.4 M), (b)Cds-II (0.6 M), (c)Cds-III(0.8), (d)Cds-IV(1.0M)

### Thermogravimetric Analyses:

TGA study Figure 3 shows a representative thermogram of Cds sample This thermogram is divided into two regions. The first weight loss (region I) is located between 337°C and 374°C and second weight loss occurs in (region II) located between 745°C and 781°C. The first derivative of this thermogram (DTG), clearly reveals the inflection points at 345°C and 750°C. The TGA decomposition patterns of cadmium sulfide, CdS nanocomposites occurs at 337°C to 374°C this is major decomposition step, The first weight loss was mainly contributed by the elimination of impurities, residual water and unreacted monomers. The second step weight loss which is attributed at 745°C to 781°C is due to the degradation of Cds nanoparticles



**Fig .3: TGA of Cds nanoparticles.**

**CONCLUSION:**

The CdS nanoparticles were successfully synthesized through Wet Chemical route method and X-ray diffraction was employed to study the structural properties, the particle sizes calculated were have zinc blende structure, from optical absorption measurement it is found that as molar concentration varies from 0.4 M to 1.0 M the band gap increases while the wavelength of absorption onset shifts to shorter wavelength. Therefore, the onset wavelength is directly related to nanoparticle size. Chemical reaction rates directly affects the time evolution of the no of nuclei, which determines both nucleation and growth process, nucleation and growth takes place simultaneously. This overlapping of nucleation and growth process, which is more pronounced as the chemical reaction is slower, leads to larger nanoparticle size. Rate of reaction depends on the molar concentration of reactants solution and increases with the increase in molar concentration of reactants solution. In the present study, the molar concentration of reactants solution varies from 0.4 M to 1.0 M, the reaction rate is highest for 1 M solution and hence the particle size obtain smallest for 1 M solution as compare to other material in the series, which is in accordance with the above Made argument. TGA results depict that the thermal stability of CdS nanocomposites showing strong interactions between the CdS nanoparticles<sup>16-18</sup>, nanocomposites are compared to their respective precursor complexes used in the synthesis of the metal sulfide nanoparticles, it could be noted that the nanocomposites are more thermally stable than their precursor complexes at temperatures below 781<sup>0</sup> C. This confirms strong interaction between metal sulfide nanoparticles

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