



# Preparation and characterizations of cadmium sulfide nanoparticles



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## ABSTRACT

Cadmium sulfide nanoparticles have been synthesized by chemical precipitation method. The X-ray diffraction patterns conform their hexagonal structure. Raman spectra show first, second and third order longitudinal optical modes, and are slightly shifted to lower wavenumber side as compared to its bulk. Optical absorption spectra of cadmium sulfide nanoparticles show that band edge is slightly shifted toward longer wavelength side (red shift) and this shift is due to the quantum confinement effect. Particle size calculated by absorption data shows quantum confinement effect. Photoluminescence shows a broad emission with peak centered at around 460 nm after excitation with 360 nm. The frequency dependent dielectric constant of cadmium sulfide nanoparticles was also investigated and normal behavior with applied field is seen. The values of real part of dielectric constant and imaginary part of dielectric constant show dispersion at low frequencies and become almost saturated at higher frequencies. The above characterizations support the quantum dot formation of cadmium sulfide by this low cost technique.

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## 1. Introduction

Semiconductor nanoparticles (NPs) have shown extra ordinary fluorescence properties and high quantum efficiency [1]. Mostly II–IV semiconductor NPs of dimensions below Bohr diameter exhibit interesting optoelectronic properties due to quantum size effect and are potential candidates for several of applications. In general with surface-area effects, quantum effects start to dominate the properties of matter as size is decreased to the nanoscale. These can have visible impact on the structural, optical, and electrical properties of materials [2]. In principle; the various properties of semiconductor materials can be varied by playing with their size and shapes. Therefore, the current research interest for condensed matter community is the preparation of semiconductor nanostructured with tuned size and shape. Cadmium sulfide (CdS) belongs to the II–VI group, a direct band gap ( $E_g = 2.42$  eV) semiconductor and is one of the promising materials for use in photoelectric conversion in solar cell [3], thin film transistor (TFT) [4], nonlinear optics [5], semiconductor laser [6] and flat panel display [7].

CdS with a room-temperature (RT) direct band gap of 2.42 eV is extremely photosensitive throughout the entire spectrum from

infra-red down to ultraviolet, which makes it a potential and attractive semiconductor in the field of optoelectronics.

In general, CdS posses three phases, in bulk form it exists in a hexagonal wurtzite-type (W) crystal structure with  $a = 0.4160$  nanometer (nm) and  $c = 0.6756$  nm but in nano crystalline phase it can have a cubical zinc blende (Z) structure and a high-pressure rock salt phase [8]. Their exist various methods for preparations CdS NPs, the solid phase [9], precipitation in the liquid phase [10] and growth in nano-sized micells [11]. However, many techniques for the synthesis of CdS nano-crystals have been developed but a challenge still exists to synthesize CdS nano-crystals in the quantum confinement range. Therefore, here we discuss a simple chemical precipitation technique to synthesize CdS nano particles.

## 2. Experimental

CdS NPs are prepared by precipitation technique from  $\text{CdSO}_4$ , using thiourea and  $\text{NH}_4\text{OH}$ . All the chemicals are of AR grade from Merck Ltd. In this work, NPs are prepared by mixing aqueous solution of  $\text{CdSO}_4$  of 0.1 M concentration with aqueous solution of thiourea 0.02 M concentration. The pH of the mixture solution is kept at 10 by adding  $\text{NH}_4\text{OH}$ . The mixture stirred for 1 h. Then this mixture was sonicated (with 50 W power and 40 kHz operational frequency) at room temperature for 1 h. The color of the solution changed to yellow and precipitation occurs. The precipitated

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CdS NPs are filtered, washed, dried and then used for different characterizations.

These CdS NPs were characterized by X-ray diffraction (XRD) with Cu K $\alpha$  radiation ( $\lambda = 1.5418 \text{ \AA}$ ) using Rigaku Rotating Anode (H-3R) diffractometer. The surface morphology of the NPs was carried out using high resolution Field Emission Scanning Electron Microscope (FESEM, S-4300, Hitachi, Japan). The UV–vis spectroscopy of the samples was studied by using Shimadzu UV-1650 spectrometer. Photoluminescence (PL) was done Shimadzu spectrofluorometer RF-5301. Fourier Transform Infrared (FT-IR) spectrum was recorded on Perkin-Elmer Paragon-1000 spectrophotometer Esquire 3000 spectrometer by KBr pallet technique. Raman measurements were carried out by using Renishaw InVia Raman microscope. The Argon (Ar) laser (514 nm) was used for excitation and the laser power was kept 1 milli Watt (mW), with 20 $\times$  objective. The dielectric study of CdS NPs was studied in the 40 Hz–1 MHz frequency range using with an Agilent 4285A precision Inductance Capacitance Resistance (LCR) meter. The dielectric constant and dielectric loss were studied by parallel plate geometry method (the pellets of these NPs were polished by silver paint to form the conducting electrodes). All the above characterizations were done at 300 K.

### 3. Results and discussions

Fig. 1 shows the XRD pattern of CdS NPs. Several peaks of hexagonal phase with  $a=b=4.136 \text{ \AA}$ ,  $c=6.713 \text{ \AA}$  (wurtzite-type structure), have been obtained due to diffraction from (100), (002), (111), (102), (110), (103), (112) and (203) planes of CdS. The peaks are well matched with standard PDF card for hexagonal CdS (JCPDS file card 10-454). It is also noticed that the observed peaks are broad and which indicates nano crystalline formation of the system. The lattice parameter has been computed as  $5.29 \text{ \AA}$  which is very close to the standard value ( $5.42 \text{ \AA}$ ).

The particle size ( $L$ ) was calculated from the width of first peak using Debye Scherrer formula [12].

$$L = \frac{0.9\lambda}{\beta \cos \theta} \quad (1)$$

where  $L$  is the coherence length,  $\beta$  is full width at half maximum (FWHM) in radian of the XRD peaks,  $\theta$  is the diffraction angle and  $\lambda$  is the wavelength of X-ray used. In addition, the diameter of crystallite ( $D$ ) is given by

$$D = \frac{4}{3}L \quad (2)$$

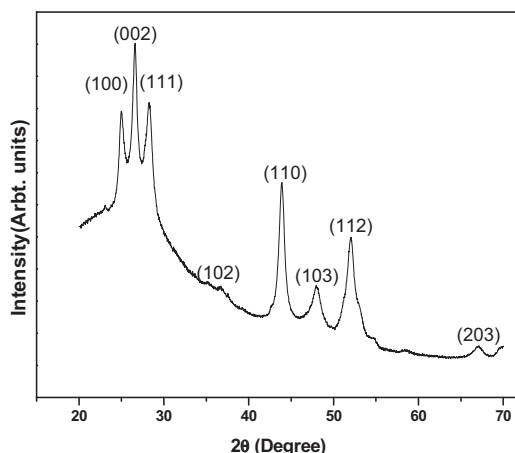


Fig. 1. XRD pattern of CdS NPs.

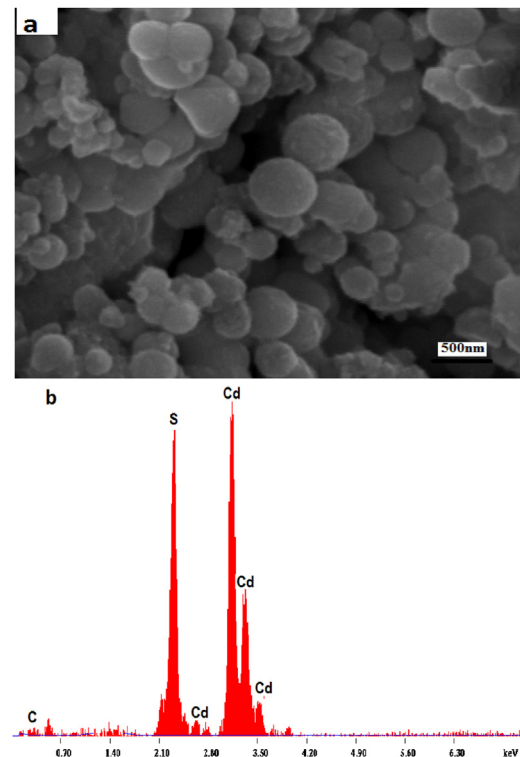


Fig. 2. (a and b) SEM and EDS images of CdS NPs respectively.

The average size calculated for samples were approximately 3.15 nm.

One can observe the line width become broader due to the decrease in grain size. Broad peaks also reflect the increase in the concentration of lattice imperfection due to the decrease in the internal micro strain within the system [12]. Smaller grain size maximizes the imperfect regions of the material, which is also supported by the smaller strain and dislocation densities.

Information on the strain and the particle size was obtained from the FWHM of the diffraction peaks. After applying the correction for instrumental broadening, the FWHM's can be expressed as a linear combination of the contributions from the strain and particle size through the following Williamson–Hall equation [12]:

$$\frac{\beta \cos \theta}{\lambda} = \frac{1}{L} + \frac{4\epsilon \sin \theta}{\lambda} \quad (3)$$

where  $\epsilon$  is the effective strain. A plot of  $(\beta \cos \theta)/\lambda$  versus  $(4 \sin \theta)/\lambda$  for this film (figure not shown here) is used to calculate the existing strain. The estimated  $\epsilon$  turns out around 0.058 which is small but quite significant. Hence force us to predict that there may be some non-uniform strain and departure from uniform shape along the different crystallographic orientations.

The surface morphology of the prepared sample can be studied by FESEM. Fig. 2a shows the FESEM image for CdS NPs. The surface of every particle is smooth and looks perfectly round shaped or spherical and are uniformly distributed over the entire scanning area. The particle size of CdS NPs as seen in the FESEM micrographs is of the order of few hundred to tens of nanometres. Fig. 2b shows the energy dispersive X-ray analysis (EDAX) of the CdS NPs. The chemical constituents present in the sample according to the EDAX results are Cd = 49.15% and S = 50.85% for CdS. This conforms the purity of the sample.

Fig. 3a shows the FTIR spectrum of CdS NPs, which shows stretching bands at 600–700, 800–950, 1000–1265, 1435  $\text{cm}^{-1}$  and 1625 due to C–S, C–C, C–O  $\text{CH}_2$  and  $\text{CO}_2$ , respectively. Hydrogen bonded stretching at 3200–3600  $\text{cm}^{-1}$  due to inter molecular

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