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Synthesis of PVA capped hexagonal CdS nanocrystals at Room temperature

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Abstract

Cadmium sulphide nanocrystals with Cd:S molar ratio 0.02:0.02 and 0.04:0.04 has been synthesized by chemical coprecipation method at room temperature using poly vinyl alcohol (PVA)as capping agent. The crystallite sizes are determined from XRD analysis. The X-ray diffraction analysis confirms that hexagonal phase cadmium sulphide nanocrystals are formed. The average crystallite sizes are found to be6 nm. From UV-visible spectra the band gap is found to be between 2.53-2.56 eV indicating a significant blue shift from it bulk band gap energy 2.42 eV.

Keyword: Nanocrystals, PVA, XRD, Band gap, UV-visible.

Introduction

CdS is a group II-VI semiconductor having a direct band gap of 2.42 eV, is of great interest due to several application in both optoelectronic and biological fields[1]. Since CdS has a wide band gap, so it is one of the most vital material among II-VI compounds for detecting visible radiation[2]. CdS is used as window material for hetero junction solar cells to avoid the recombination of photogenerated carriers which improves the solar cells efficiency[2, 3]. It is also used in light emitting diodes[4], photo detectors[5], sensors[6], address decoders[7] and electrically driven lasers[8]. Most of the II-VI compound semiconductors (e.g Zn, Cd or Hg with S, Se or Te) are found in two phases near ambient temperature and pressure; wurtzite (hexagonal) or zinc blende (cubic) [9]. It is well known that CdS generally occurs in hexagonal wurtzite phase at room temperature and can be transformed to cubic zinc blende and rock salt phases by application of suitable temperature and pressure. It is found that the rate of phase transformation from wurtzite to zinc blende increases as the temperature increases at ambient pressure and the transformation is fast in low pressure and high pressure rather than any other thermodynamic condition[10]. Moreover there is report that cubic phase CdS can be transformed to hexagonal one when heated to certain temperature[11, 12]. In this work, CdSnanocrystals having hexagonal (wurtzite) phase has been synthesized by chemical coprecipitation method at room temperature using PVA as capping agent. Structural analyses are carried out by XRD and TEM, whereas optical analyses are observed by UV-visible spectra.

Methodology

Synthesis: CdSnanocrystals are prepared by chemical coprecipation method. 0.02 M and 0.04 M $CdCl_2$ and same amount of Na_2S are prepared separately in 20 ml triple distilled water. 4% PVA (Polyvinyl alcohol) is prepared separately and mixed with $CdCl_2$ solutions. The solutions are then mixed together and stirred which are kept undisturbed for 24 hours. The precipitates are filtered and rinsed with triple distilled water for several times so that the foreign particles are removed. The precipitates are than kept in room temperature for some days to dry and then grinded to obtain in powder form. The samples are ready for characterization. The powders are characterized by X-ray diffractometer (D8 Advance, Bruker AXS) with CuK_α radiation (λ=0.15406 nm), UV-visible spectra (Carry 300 spectrophotometer) and transmission electron microscope (JEM-2100, Jeol).

Result and Discussion

Structural investigations are carried out using X-ray diffractometer. Figure-1 shows the X-ray diffraction pattern of CdS powder with Cd:S molar ratios of (a) 0.02:0.02 and (b) 0.04:0.04 M respectively. The XRD pattern of samples (a) and (b) exhibit three prominent peaks at 2Θ values at 25.57^0, 26.72^0, 27.77^0, 44.13^0, 47.89^0, 52.24^0 and 71.35^0corresponding to the diffraction from (100), (002), (101), (110), (103), (112) and (211) planes respectively of hexagonal wurtzite phase of CdS (JCPDS card no. 77-2306). Another important feature of the XRD pattern is that (100), (002) and (101) are superimposed and they have to be separated for X-ray peak profile analysis. These peaks are decomposed to individual peaks by considering Lorentziandistribution for each component peak. Figure-2 shows the decomposed of the three peaks corresponding to the plane (100), (002) and (101). The broadening of different peaks of nanoparticles is obviously the characteristic of nanosized particles[13]. The crystallite size are calculated according to Scherrer formula

$$t = K.\lambda / (\beta \cos\Theta) \quad (1)$$

Where K is a constant and its value is 0.9, λ is the wavelength of radiation which is 1.5406 A^0 for CuK_α radiation, β (in radian) is the full width half maximum (FWHM) of the peaks and Θ is the Braggs diffraction angle[14, 15, 16]. The average crystallite size is found to be 6 nm which is in good agreement with the TEM

image as shown in figure-3. The crystallite size for each plane as well as the average crystallite size of all the planes for each sample is shown in Table-1. In order to further investigate the microstructural properties, TEM characterization is carried out on the CdS nanocrystals. Figure-3 shows the TEM micrograph of the nanocrystals. Nanocrystals of size about 8nm having nearly spherical shape can be clearly seen from the HRTEM micrographs. The optical properties are carried out with help of UV-visible spectra which is shown in the figure-4. The optical band gap values of the samples are presented in table-2. The UV-visible spectra show a blue shift which is shown in Figure-4. This blue-shift also confirms the nanocrystalline nature of the samples and is caused by the strong quantum size effect in nanoparticles[17]. The absorption edge shifts towards lower wavelength side (blue region) as the molar ratio of Cd:S decreases indicating that the effective band gap energy increases with the decrease in particle size.

Table-1
Crystallite size (nm) of the samples of CdS nanoparticles

Samples	Molarity of Cd:S	Planes (hkl)	Crystallite size (nm)	Average Crystallite Size(nm)
(a)	0.02:0.02	(100)	5.619508	6.018
		(002)	6.6282	
		(101)	6.889912	
		(110)	5.913405	
		(103)	5.559403	
		(112)	5.713106	
		(211)	5.689188	
(b)	0.04:0.04	(100)	5.469919	6.0258
		(002)	6.609364	
		(101)	6.839863	
		(110)	5.963697	
		(103)	5.397881	
		(112)	5.861837	
		(211)	6.038444	

Table-2
Band gap (eV) of the samples of CdS nanoparticles

Samples	Molarity of Cd:S	Band gap energy (eV)
(a)	0.02:0.02	2.56
(b)	0.04:0.04	2.53

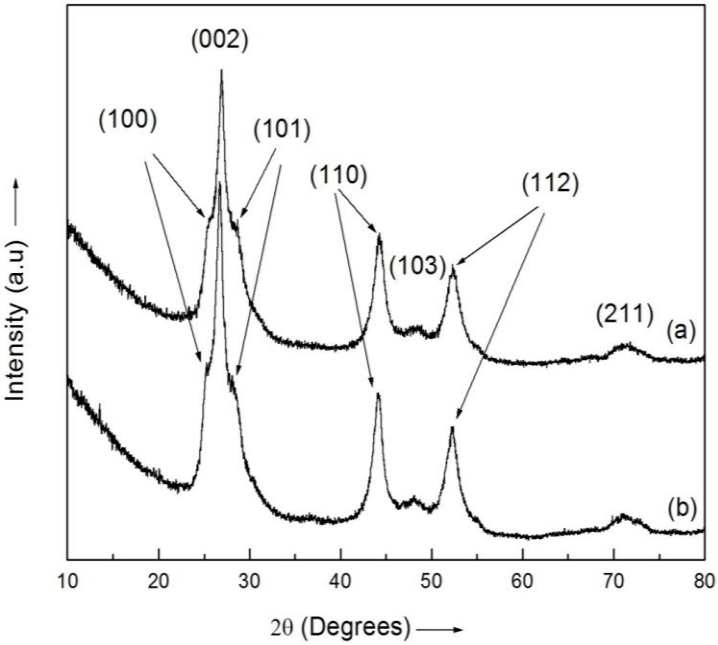

Figure-1
XRD pattern of CdS powder with Cd:S molar ratio (a) 0.02:0.02 (b) 0.04:0.04

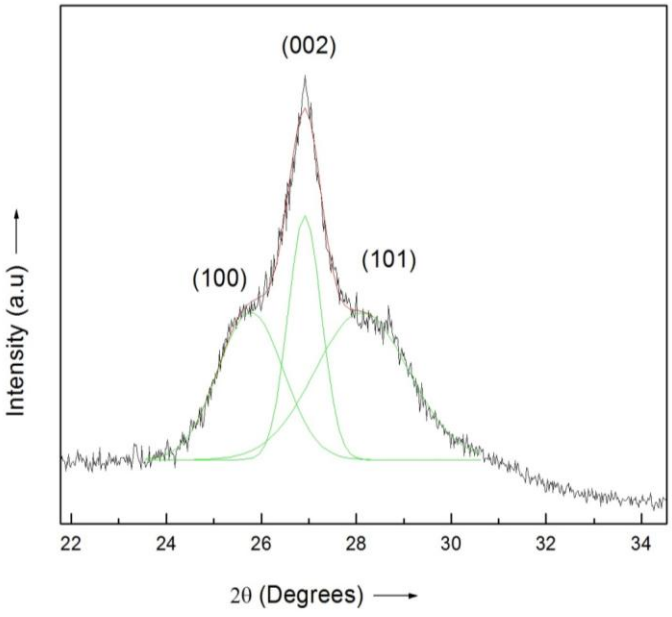

Figure-2
Decomposition of the peaks from planes (100), (002) and (101)

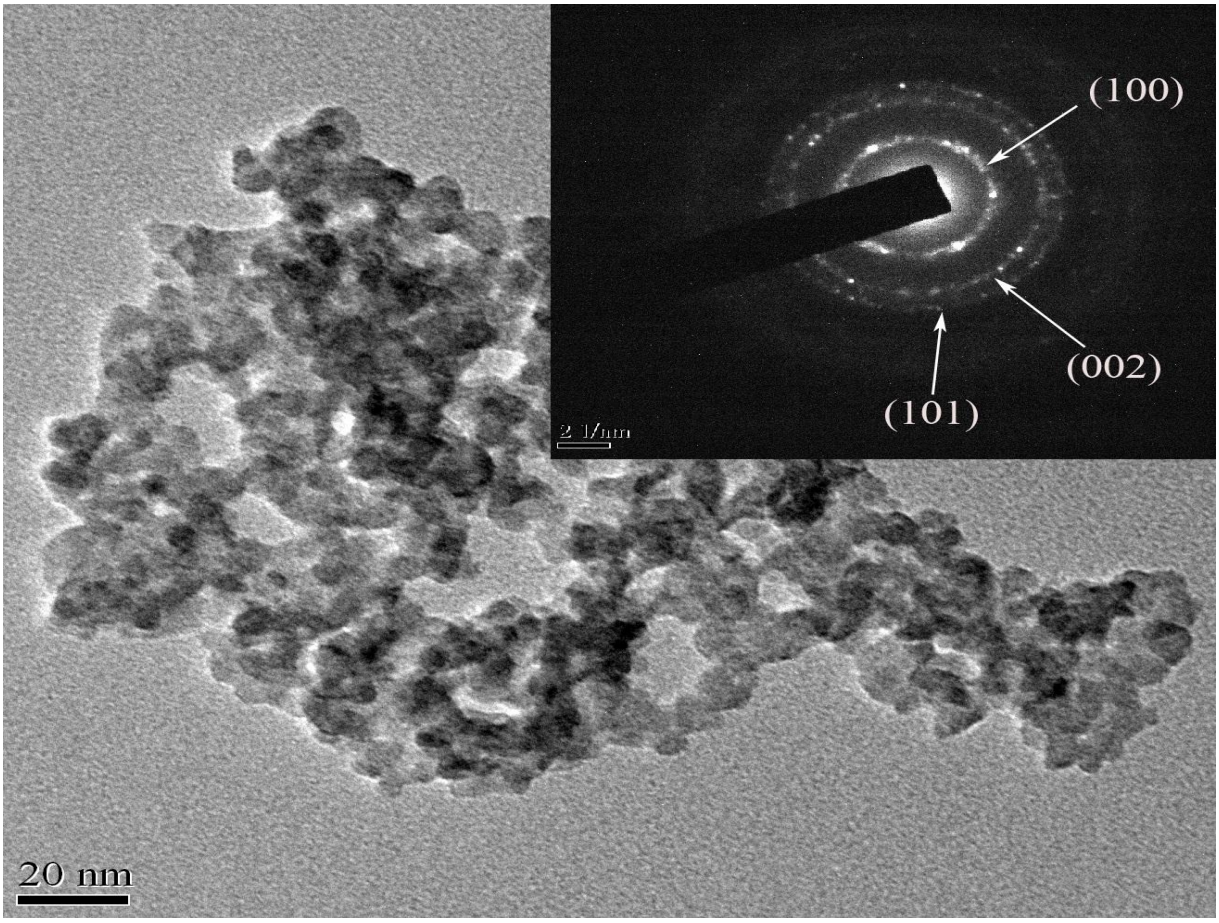

Figure-3
HRTEM image of CdS nanocrystals along with its SAED pattern

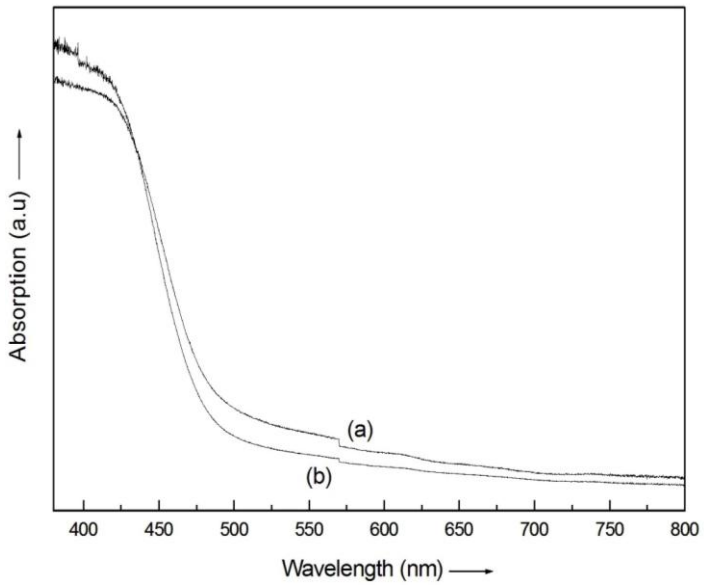

Figure 4
UV –visible spectra of CdS with Cd:S molar ratio (a) 0.02:0.02 (b) 0.04:0.04

Conclusion

In summary, CdS nanocrystals have been successfully synthesized by chemical coprecipitation method at room temperature with varying Cd:S molar ratio having hexagonal phase. XRD analysis reveals that the prepared CdS samples are of hexagonal wurtzite structure and well crystalline nature. The average crystallite sizes are found to be 6.35 nm which is in good agreement with the TEM image. The morphology and particle size distribution has been studied by transmission electron microscopy (TEM). The UV-visible spectra show a blue shift. With the increase of Cd:S molar ratio the band gap of the samples decreases.

References

1. Chen Q., Bao H. and Shen X., Phase transition of CdS in the presence of ethylenediamine and formation of hollow CdS submicron particles with needle-like structure, *Phase trans.*, **81,** 591-601(**2008**)

2. Singh V. and Chauhan P., Synthesis and structural properties of wurtzitetype CdS nanoparticles, *Chalc. Lett.*, **6(8)** 421-426 (**2009**)

3. Morales-Acevedo A., Thin film CdS/CdTe solar cells: Research perspectives, *Sol. Ener.* doi:10.1016/ j.solener.2005.10.008 (**2005**)

4. Murai H., Abe T., Matsuda J., Sato H., Chiba S. and Kashiwaba Y., Improvement in the light emission characteristics of CdS: Cu/CdS diodes, *Appl. Surf. Sci.*, **244,** 351(**2005**)

5. Wang Y., Ramanathan S., Fan Q., Yun F., Morkoe H. and Bandyopadhyay S., Electric Field Modulation of Infrared Absorption at Room Temperature in Electrochemically Self Assembled Quantum Dots, *J. Nanosci. Nanotechnol*. **6(7)** 2077-2080 (**2006**)

6. Ponzoni A., Comini E., Sbervcglieri G., Zhou J., Deng Z.S., Xu N.S., Ding Y. and Wang Z.L, Ultrasensitive and highly selective gas sensors using three-dimensional tungsten oxide nanowire networks, *Appl. Phys. Lett*., **88,** 203101 (**2006**)

7. Zhong Z.H., Wang D.L., Cui Y., Bockrath M.W. and Lieber M.C, Nanowire Crossbar Arrays as Address Decoders for Integrated Nanosystems, *Science*, **302,** 1377-1379 (**2003**)

8. Duan X., Huang Y., Agarwal R. and Lieber C.M., Single-nanowire electrically driven lasers, *Nature*, **421,** 241-245 (**2003**)

9. Kelley A.M., Dai Q., Jiang Z., Baker J.A. and Kelley D.F., Resonance Raman spectra of wurtzite and zincblende CdSenanocrystals, Chem. Phys., **422,** 272-276 (**2013**)

10. Ghosh A., Paul S. and Raj S., Structural phase transformation from wurtzite to zinc-blende in uncapped CdS nanoparticles, *Sol. Stat. Comm.*, **154,** 25-29 (**2013**)

11. Sahu N., Arora M.K., Upadhyay S.N. and Sinha A.S.K., Phase Transformation and Activity of Cadmium Sulfide Photocatalysts for Hydrogen Production from Water: Role of Adsorbed Ammonia on Cadmium Sulfate Precursor, Industrial and engineering chemistry research, **37(12),** 4682-4688 (**1998**)

12. Angel O.Z and Morales R.L, Sphalerite-wurtzite phase transformation in CdS, Phys. Rev. B **62** 13064 (**2000**)

13. Bodo B. and Kalita P.K., Structural and Optical Properties of ZnS:Cu Transparent Nanosheets, *Res. J. Physical Sci.*, **1(1)** 2-5 (**2013**)

14. Kumar A.G., Reddy R.V.M. and Reddy N.K, Structural, Optical and Electrical Characteristics of Nanostructured ZnO Thin Films with various Thicknesses deposited by RF Magnetron Sputtering, *Res. J. Physical Sci.*, **1(6),** 17-23(**2013**)

15. Senapati U.S., Jha D.K. and Sarkar D, Green Synthesis and Characterization of ZnS nanoparticles, *Res. J. Physical Sci.*, **1(7)** 1-6 (**2013**)

16. Sivaraman T., Nagarethinam V.S. and Balu A.R., CdS thin films Fabricated by a simplified Spray technique from different Substrate Temperatures – Structural, Morphological, Optical and Electrical analysis, *Res. J. Mater. Sci.* **2(2)** 6-15 (**2014**)

17. Harish G.S., Divya A., Kumar S.K. and Reddy S.P., Synthesis and Characterization of Water Soluble ZnS: Ce, Cu co-Doped Nanoparticles: Effect of Polyvinyl Alcohol Concentration, *Res. J. Physical Sci.*, **1(7),** 7-10 (**2013**)