Research Journal of Physical Sciences _____ ISSN 2320–4796
Vol. **2(7),** 1-3, December **(2014)** *Res. J. Physical Sci.*

Synthesis and Characterization of PVA capped CdS nanocrystals

Deka Kuldeep
Department of Physics, Gauhati University, Guwahati-781014, Assam, INDIA

Available online at: www.isca.in
Received 14th November 2014, revised 21st November 2014, accepted 2nd December 2014

Abstract

Cadmium sulphide (CdS) nanocrystals with Cd:S molar ratio of 0.2:0.2, 0.3:0.3, 0.4:0.4, 0.5:0.5 M are synthesized by chemical coprecipitation method using poly vinyl alcohol (PVA) as capping agent. Crystallite sizes of CdS nanocrystals are determined from XRD analysis. The crystallite sizes are found to be 3.34, 3.54, 3.75, 4.18 nm for molarity 0.2, 0.3, 0.4, 0.5 M respectively. The X-ray diffraction pattern study confirms that cubic phase cadmium sulphide nanocrystals are formed. From UV- visible spectra the band gap is found to be lying between 2.7-2.9 eV indicating a significant blue shift from its bulk of band gap energy 2.42 eV.

Keyword: Nanocrystals, Crystallite size, PVA, XRDand UV-visible.

Introduction

CdS is a group II-VI semiconductor with a direct band gap of 2.42 eV, which is of great interest due to their several applications in both optoelectronic and biological fields[1]. Due to its wide band gap, it is one of the most vital materials among II-VI compounds for detecting visible radiation[2]. CdS is also 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]. It exists in cubic (sphalerite), hexagonal (wurtzite), orthorhombic or their mixed crystalline phases[9-13]. In order to understand the various physical, chemical or mechanical properties of nanocrystals, different structural aspects must be considered and thereby proper estimation of structural parameters like crystallite size, lattice strain, stress, energy density etc. are important. In the present work, CdS nanocrystals having cubic (zinc blende) phase has been synthesized by chemical coprecipatition method. Structural analysis has been done by XRD and TEM analysis and optical properties are observed by UV- visible spectra.

Methodology

Synthesis: CdS nanocrystals are prepared by chemical coprecipation method. 0.2 M, 0.3 M, 0.4 M, 0.5 M $CdCl_2$ and same amount of Na_2S are prepared separately in 20 ml triple distilled water. 2% 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 heated up to 70^0 C to dry and then grinded to obtain in powder form. The samples are ready for characterization. The powders are characterized by X-ray diffract meter (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).

Results and Discussion

Structural investigations are carried out using X-ray diffractmeter. Figure-1 shows the X-ray diffraction pattern of CdS powder with Cd:S molar ratios of 0.2:0.2 (a), 0.3:0.3 (b), 0.4:0.4 (c) and 0.5:0.5 (d) M respectively. The XRD pattern of samples (a), (b),(c) & (d) exhibit three prominent peaks at 2Θ values at 26.91^0, 44.17^0 and 52.04^0 corresponding to the diffraction from (111), (220) and (311) planes respectively of cubic zinc blende phase of CdS (JCPDS card no. 89-0440). The broadening of different peaks of nanoparticles is obviously the characteristic of nanosized particles[14]. 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[15, 16]. The average crystallite size is found to be 3.7 nm which is in good agreement with the TEM image as shown in figure-2. 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 micro structural properties, TEM characterization is carried out on the CdS nanocrystals. Figure-2 shows the TEM micrograph of the nanocrystals. Nancrystals of size about 4nm 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-3. 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-3. 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)	0.2:0.2	(111) (220) (311)	4.437 4.25 3.866	4.184
(b)	0.3:0.3	(111) (220) (311)	3.931 3.769 3.551	3.75
(c)	0.4:0.4	(111) (220) (311)	3.714 3.565 3.363	3.547
(d)	0.5:0.5	(111) (220) (311)	3.444 3.409 3.194	3.349

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

Samples	Molarity of Cd:S	Band gap energy (eV)
(a)	0.5:0.5	2.7
(b)	0.4:0.4	2.73
(c)	0.3:0.3	2.9
(d)	0.2:0.2	2.93

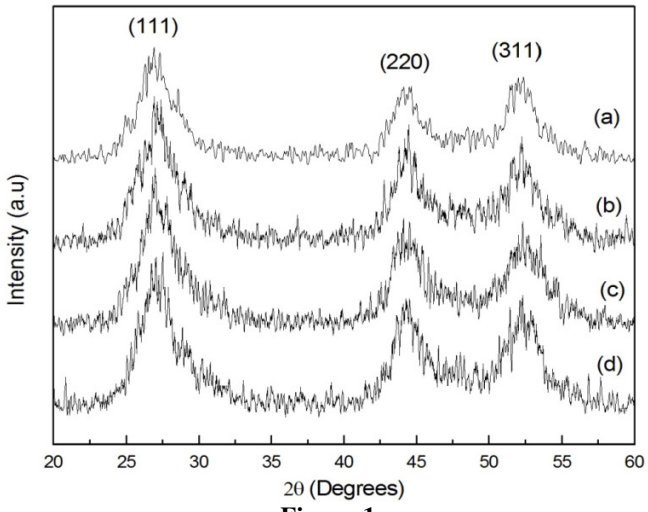

Figure-1
XRD pattern of CdS powder with Cd:S molar ratio (a) 0.2:0.2 (b) 0.3:0.3 (c) 0.4:0.4 (d) 0.5:0.5

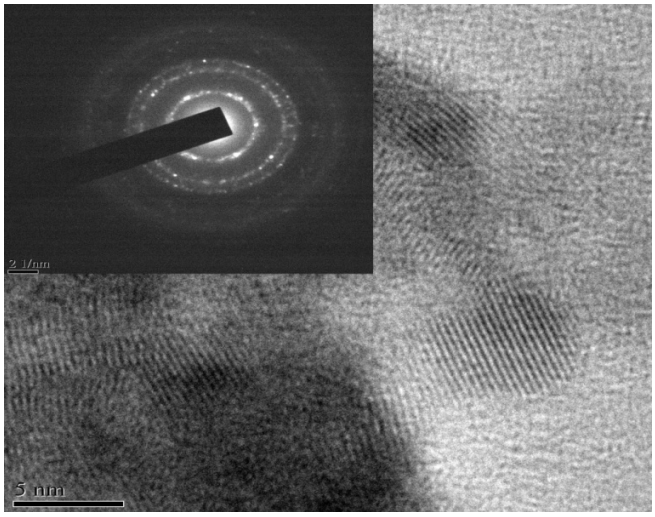

Figure-2
HRTEM image of 0.5 M CdS along with its SAED pattern

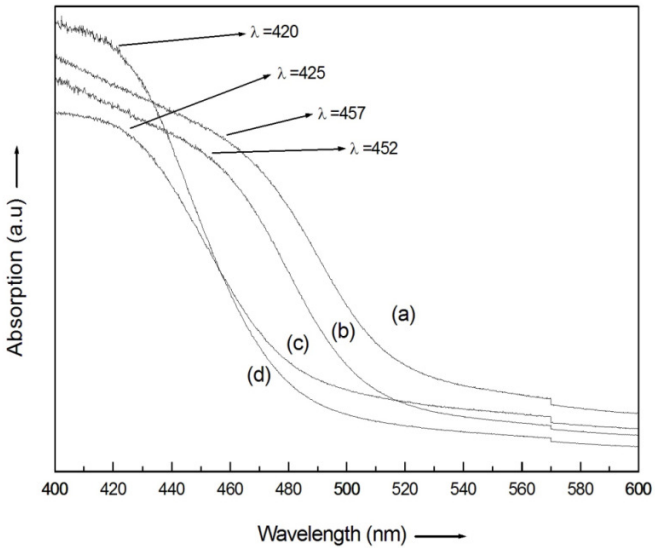

Figure-3
UV –visible spectra of CdS with Cd:S molar ratio (a) 0.5:0.5 (b) 0.4:0.4 (c) 0.3:0.3 (d) 0.2:0.2

Conclusion

In summary, CdS nanocrystalshave been successfully synthesized by chemical coprecipitation method with varying Cd:S molar ratio. XRD analysis reveals that the prepared CdS samples are of cubic zinc blende structure and well crystalline nature. The average crystallite sizes are found to be 3.7 nm which is in good contrast 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., Chauhan P., Synthesis and structural properties of wurtzitetypeCdS 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 inElectrochemically 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. Kizilyalli M., Bilgin M., Usanmaz A., Synthesis of a new orthorhombic metastable form of CdS through solid-state reactions, *J. Sol. Stat. Chem*., **80** 75-79(**1989**)

10. Li X., Zhang H., Gao J., Guo D., Yang C., Xu L., Liu B., Zhang X.,Transition temperature reduction for CdS nanoparticles under high pressure, *J. Nanopart. Res*., **13** 6563-6568(**2011**)

11. Benkhettou N., Rached D., Soudini B., Driz M., High-pressure stability and structural properties of CdS and CdSe, *Phys. Status. Sol B,* **24** 101-107(**2003**)

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

13. Du Y., Zeng F., Solvothermal route to CdSnanocrystals, *J. Exp. Nanosci*., **8** 965-970(**2013**)

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

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

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

17. Harish G.S., Divya A., Kumar S.K., 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**)