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RESEARCH ARTICLE

Structural and Spectroscopic Studies of Chalcogenide Nano Particles

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Abstract

CdSe Nano particles were grown by Chemical Bath Deposition. The pH of the solution was maintained at 11. The precipitate so obtained was annealed in air for about 4 hours at 300^0C temperature. The annealed powdered samples were subjected to optical and structural characterization using UV-Visual spectrophotometer, Raman and XRD. Powdered XRD was used for structural characterization whereas UV-Visual and Raman spectroscopy were used for optical characterization. XRD spectra reveals that the grown CdSe nano particles are polycrystalline in nature and have hexagonal structure. The average particle size, using Debye-Scherer formula, in CdSe powdered sample was found to be of the order of 4.5nm. UV-Visual transmittance spectra recorded over the wavelength range 350 to 900 nm and Tau plots were used to calculate the band gap of CdSe Nano particles. It was found that the band gap is 1.7eV. Raman spectra of annealed CdSe powder shows that polycrystalline nature of the sample in nanocrystalline regime. Reported result shows that the Raman shift should decrease with an increase in nanocrystallite size.

INTRODUCTION

Presently nanoparticle materials have opened field of electronic applications, since material properties could be changed by changing the nanoparticle size and/or thickness of the film. New applications in various fields are also emerging. Development of such materials, whose structural, electrical and optical properties could be controlled, will be useful in many ways.

For example optoelectronic devices, particularly solar energy conversion devices could be modified accordingly. The synthesis of binary metal chalcogenide of groups II-VI semiconductors in a nanoparticle form has been a rapidly growing area of research due to their physical and chemical properties .CdSe nanoparticles have been prepared by various techniques including chemical bath deposition (CBD) . CBD is a well-known method for preparing semiconductor and has been used mainly for metal selenides.CdSe is a chalcogenide compound, which belongs to Group II-VI semiconductors family. CdSe is n–type semiconductor with a band gap (Eg) of 2.64 eV at room temperature.

Material and Methods

All the chemicals used in this investigation were analytical reagent grade. Metal precursor, cadmium acetate $(Cd(CH_3COO)_2.2H_2O$, selenium metal powder and sodium sulphide were procured from scientific .double distilled water used as solvent.

In the present study nano particles were synthesized at mild reaction temperature 80 °C. The basic idea of deposition is a reaction between a slowly released selenide anion with a free metal cadmium cation (Cd2+). As precursor of selenide ions (Se2-), sodium selenosulphate (Na_2SeSO_3) was used.The PH of solutions were maintained around 11.sodium selenosulphate, was used in the form of solution. 25 ml of 1 M cadmium acetate solution was taken in a 100 ml capacity glass beaker and to it, 5 ml of triethanol amine, 25 ml of 25% ammonia and 15 ml and 0.5M of sodium selenosulphate was slowly added with constant stirring. The pH of the solution was maintained at 11. The precipitate so obtained was annealed in air for about 4 hours at 300^0C temperature. CdSe nano particles are shown in figure(1).

Fig-(1) CdSe nano particles NPs

Result and Discussion

1. XRDs were recorded using diffractrometer available at SAIF in Chandigarh. Cu $-K_\alpha$ radiation of wavelength 1.54A^0 was used to record XRD. The data were recorded by scanning 2Θ from 20^o to 80^o. The peaks are detected at 2Θ values equal to 25.73°, 42.27° and 49.79°, respectively. XRD results show the presence of hexagonal phases in CdSe nano particles. They were ascribed due to (111), (110), (112) plane of hexagonal CdSe structure.The average particle size, using Debye-Scherer formula, in CdSe powdered sample was found to be of the order of 4.5nm. Average lattice constant for the CdSe nanoparticles is 6.071.

Table-1 XRD data for CdSe nanoparticles using Cu-Kα radiation

S.N.	Observed d-value	hkl plane	2Θ
1.	3.514	111	25.53
2.	2.113	110	41.10
3.	1.8286	112	49.86

2. The optical properties of CdSe nano particles deposited by using chemical bath deposition (CBD) technique using UV-VIS spectroscopy. The optical band gap of the samples is determined by the following Tauc relationship,

$$(\alpha h\nu) = A(h\nu - E_g)^m$$

From Fig 2(a),(b) UV-VIS transmission spectra of CdSe powder in the wavelength range 400 to 1000 nm were recorded. For Optical study was observed that the Energy band gap of CdSe nanoparticles (NPs) was to be found 1.7eV after annealing (2 hours at 300 degree centigrat).

3. Raman spectra of annealed CdSe powder show peak having highest intensity corresponding to dominating longitudinal optical (1LO) phonon peak at 206 cm−1. The observed (1LO) phonon peak is slightly below the bulk 1LO phonon frequency (211 cm−1). This might be due to the polycrystalline nature of the sample in nanocrystalline regime. Reported result shows that the Raman shift should decrease with an increase in nanocrystallite size. Multiphonon replicas or overtones (2LO, 3LO) were also observed with decreasing intensity in Raman Spectra. Thus Raman spectra provide confirmation to the formation of nanocrystalline CdSe nano particles.

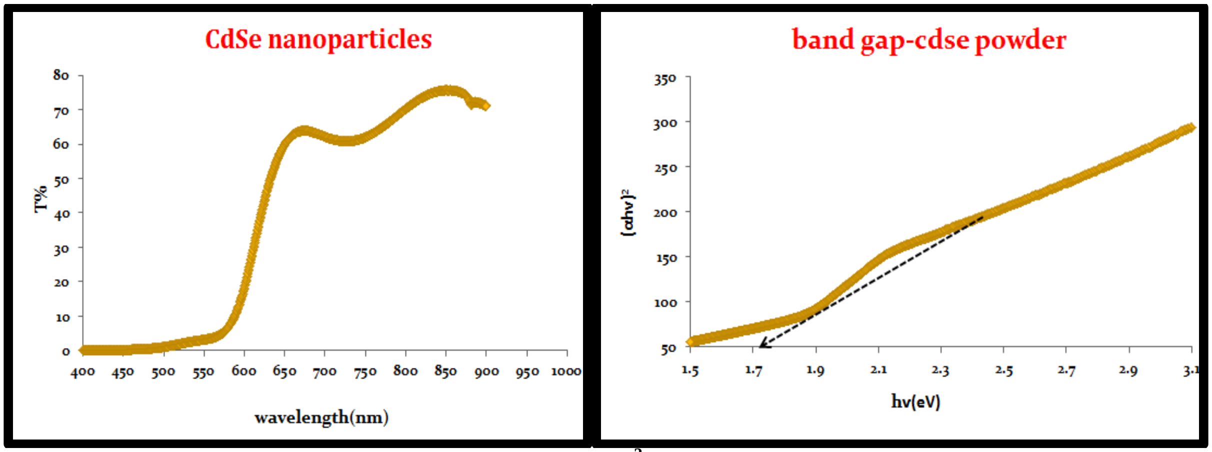

Fig.2(a),(b) Transmission spectra and Plots of $(\alpha h\upsilon)^2$ vs. hυ of CdSe nanoparticles(Nps)

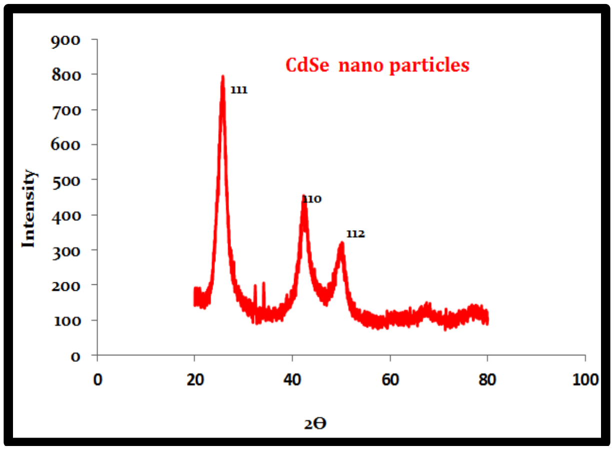

Fig.3(a), XRD Pattern of CdSe NPs

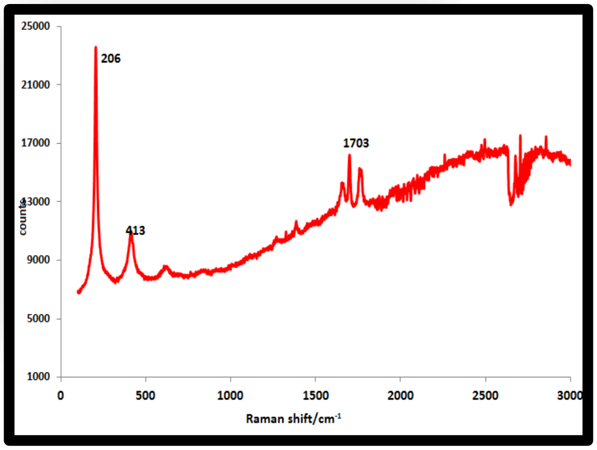

Fig.4(a) Raman spectra of CdSe(NPs)

CONCLUSIONS

CdSe Nano particles were successfully synthesized by using Chemical Bath Deposition. XRD spectra confirm that the grown CdSe nano particles are polycrystalline in nature and have hexagonal structure. Optical studies were found that the band gap is 1.7eV. Reported results confirm that the Raman shift should decrease with an increase in nanocrystallite size.

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