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Study of Optical and Structural Characteristics of PVA Capped CdS Nanoparticles

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ABSTRACT: In this report we give a simple and less hazardous route for the synthesis of CdS nanoparticles.CdS nanoparticles were synthesized using chemical reaction method at temperature 60^0C using $CdCl_2$, Na_2S as precursors. The structural and optical properties of resulting CdSnanoparticles were investigated by X-ray diffraction (XRD), Scanning Electron Microscope (SEM), Ultraviolet-visible (UV-vis) spectroscopy and Photoluminescence (PL) spectroscopy etc.The UV-vis absorption spectra shows blue shift of the absorptionedge compared to bulk CdS. SEM image reveals the shape of the formation of CdS nanoparticles is more or less spherical. The band gap value was calculated using Tauc's plot from the UV-visible spectra.

Keyword: Absorption edge, blue shift, bulk materials, Tauc's plot.

I. INTRODUCTION:

Now a days, the field of Nanoscience and Technology is one of the most important and exciting field of research, not only under the domain of Physics, but also under Chemistry, Engineering, and Medicine [1]. Nanotechnology concerns with material structures and systems whose components exhibit novel and significantly modified physical, chemical and biological properties due to their nanoscale sizes. The principal goal of Nanotechnology is to control and exploit these properties in structures and devices, at atomic, molecular and supramolecular levels. To realize this goal, it is necessary to learn to fabricate and use nanostructure efficiently [2]. With recent advances in the field of Nanotechnology, dimensions of semiconductor devices and integrated circuits are decreasing. This miniaturization in the dimensions of devices has resulted in new and advanced functions, which have made electronics more reliable, faster, more powerful and less expensive. The prefix nano means 10^{-9}i.e. one nanometer denotes one billionth of a meter. Thus, the dimensions of the devicesshould be thousand times smaller in nanoelectronics than those of microelectronics.Nanotechnology is the fabrication of nanometer sized materials called nanomaterials. At the nanometer scale of size, classical description of solidstate properties break down and quantum mechanics comes into the picture. In bulk materials, particle motion takes place in all three dimensions whereas the movement of particle is confined or restricted in one or more dimensions in low dimensional structure i.e. in nano structure. Due to such restriction or confinement of charge carriers, the electronic structure as well as electronic properties of bulk and nanostructures of the same material differs dramatically [3].

CdS is a group of II-VI semiconductor material possessing a direct band gap of 2.42 eV. It is yellow in colour. The main application of CdS nanoparticles is as a pigment. It exists in two different polymorphs which are hexagonal greenockite and cubic hawleyite. It is used in the production of solar cells where it is used as the buffer layer in the manufacture of CIGS(Copper-Indium-Gallium- Selenide).CdS nanoparticles can be used in electronic and opto electronic devices.

II. EXPERIMENTAL DETAIL

2.1 materials

All the chemicals viz Cadmium Chloride ($CdCl_2$), Sodium Sulphide (Na_2S) were of analytical grade and all were purchased from Sigma-Aldrich/Merck and were directly used without further purification. Double distilled water was used as the solvent throughout the synthesis process.

2.2 methods

In our experiment, Cadmium Sulfide nanoparticles have been synthesized usinga simplewet chemical method involving a reaction

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between the solutions of Cadmium Chloride ($CdCl_2$) and Sodium Sulfide (Na_2S). Polyvinyl Alcohol (PVA) was used as the capping agent throughout the reaction. At first 1 gm of PVA was mixed in 100 ml distilled water. The solution was then stirred for three hours until it became clear. Then, solution of 1gm of $CdCl_2$ and 1 gm of Na_2S were separately prepared by stirring for about half an hour in 100 ml distilled water. After that solutions of PVA and $CdCl_2$ weremixedin theratio of (PVA): ($CdCl_2$) = 2:1.To this solution Na_2S was added dropwise and thecolour change was observed until it turns into yellow from orange.

III. CHARACTERIZATION METHODS ADOPTED:

The synthesized samples was characterized using different characterization techniques. The room temperature photoluminescence spectra were measured using Hitachi F-2500 Photoluminescence spectrophotometerwith excitation wavelength 300 nm. UV-visible spectra were analyzed using UV-visible spectrometer. X-ray diffraction pattern was recorded with Philips X-ray diffractometer with CuK_α radiation (λ=1.546A^0) in terms of intensity versus 2θ plots with 2θ ranging from 4^0- 100^0. The morphology of the sample was studied using Scanning Electron Microscope [Model no Sigma 300]. Moreover to study the presence of element EDAX analysis was also performed.

Reaction Mechanism:

$PVOH + CdCl_2 + Na_2S \rightarrow PVOH+CdS+2NaCl$-----(1)

IV. RESULTS AND DISCUSSIONS:

4.1 XRD results:

X- ray diffraction spectra of the synthesized CdS sample was shown in the following figure. The diffraction peaks for the CdS nanoparticles are obtained at angles 2θ= 26.60^0, 44.30^0 and 52.16^0 corresponding to the reflection angles (100), (220) and (311) respectivelywhich shows the cubic zinc blende phase of synthesized CdSsample. The average crystallite samples was calculated using the De-bye Scherrer's formula which is:

$$D = \frac{K\lambda}{\beta \cos\theta} \quad \text{-------(2)}$$

where β is the full-width at half maximum (FWHM) of a diffraction peak, K = 0.9, θ is the Bragg's angle and λ is thewavelength (=1.54A^0) of CuK_α radiation. The average particle size for CdSsample was found to be 11.52 nm.

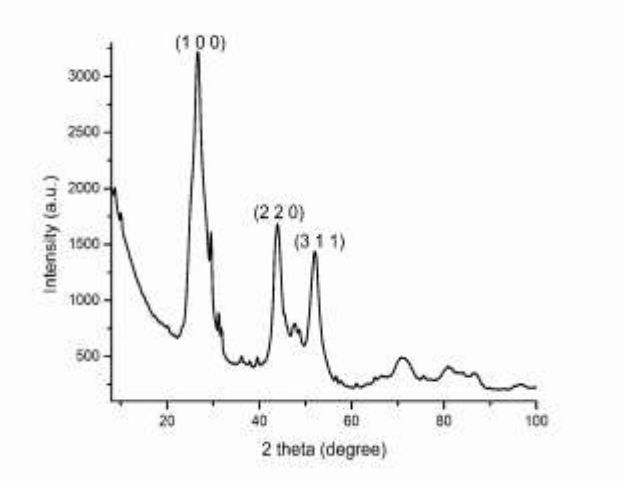

Fig 1: XRD spectra of CdS nanoparticles

4.2 SEM results:

The following figure shows the SEM images of prepared core CdS nanoparticles. From the images we can confirm that the particles are more or less spherical in shape and the size of the particles ranges from 25 to 68 nm.

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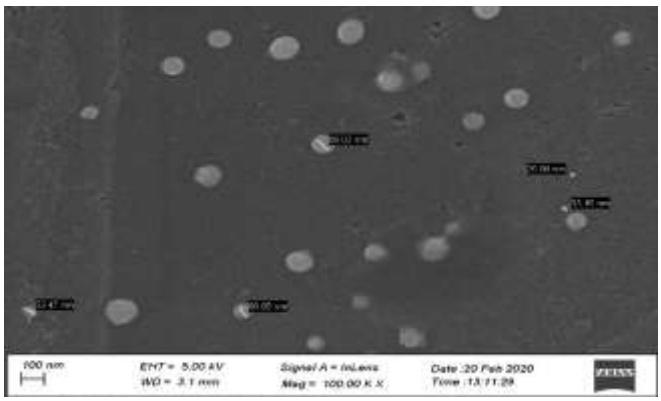

Fig2:SEM image of synthesized CdSnanoparticles

4.3 EDAX analysis

The energy dispersive X-ray spectroscopy (EDS) spectrum of the as prepared CdS sample is shown in the figure below. It indicates the presence of chemical composition of CdSnanoparticles is Cd, S etc. Other elements like Ca, O, Na, Cl, Si etc. are also revealed from the EDAX image. This confirms the elemental composition of the sample. Si and O may result from the glass slide used as a substrate for the deposition of the prepared CdS sample. Rest of the elements may be due to the coating of the semiconductor nanomaterials.

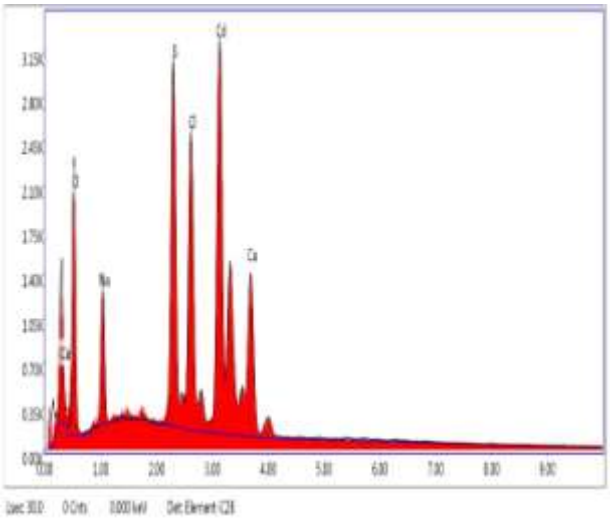

Fig 3: EDAX spectra of synthesized CdS nanoparticles

4.4Results of UV-visible spectroscopy:

UV-Vis absorption spectra of the synthesized samples was shown in the Fig. The absorption edge of CdSsamplewas found to be at 318.00 nm, which shows a clear blue shift from its bulk value of 512 nm. The energy band gap value forCdS has been estimated using the Tauc's relation given in equation$\alpha h\nu = (h\nu - E_g)^n$ ……..(3)

Here, α is the absorption coefficient, hν is the energy of incident light, E_g= Energy band gap of the material, the value of n depends onnature of the transition. For direct and indirect transitions it is ½ and 2 respectively [4]. It is seen that the band gap value for CdS nanoparticles is 4.22 eV than the band gap value of bulk CdS which is 2.42 eV, thereby confirming the formation of nanoparticles ofCdS. The absorption spectra and Tauc's plot of the CdS sampleare shown in Fig 4 and Fig 5 respectively.

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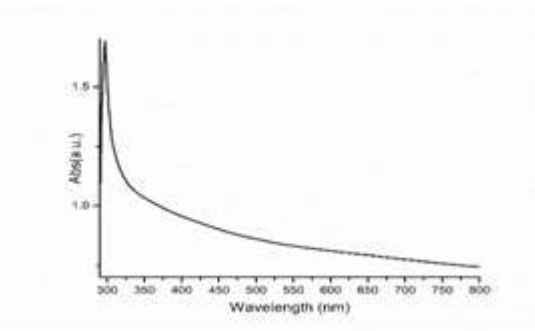

Fig4: Absorption spectra of CdSnanoparticles

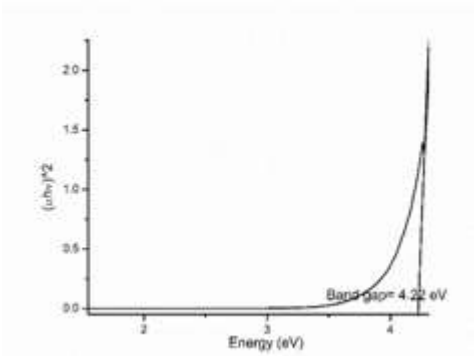

Fig 5:Tauc's plot of synthesizedCdS nanoparticles

4.5 ResultsofPhotoluminescence Spectroscopy:

The photoluminescencespectroscopyis a useful characterizationtechnique which provides useful information about the optical and photochemical characteristics of a semiconductor.The room temperature photoluminescence spectra of CdS sample is shown in the fig as follows. The excitation wavelength of CdS nanoparticles was 290 nm and the PL peak was about 323.79 nm. Another less intense peak in PL analysis was also observed at 410.28 nm.This emission in the bluish range may be due to surface defect states present in the CdS sample[5].

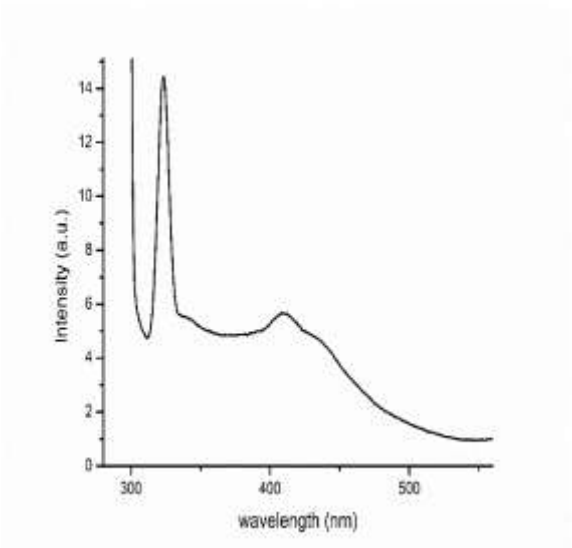

Fig 6: Photoluminescence spectra of CdS nanoparticles

V. CONCLUSION:

In summary, it can be concluded that cubicCdS nanoparticles were successfully synthesized using chemical reaction method. Formation of CdSnanoparticles have been confirmed by various characterization techniques such as UV- Visible Spectroscopy,Photoluminescence Spectroscopy, XRD, SEM, EDAX etc. The absorption edges obtained from UV-Visible spectroscopy results forCdS samples show blue shift of the absorption edges compared to the bulk value of CdS. This confirms the formation of nanoparticles of CdS. Also the bandgap values of CdS nanoparticles are larger in comparison to the bulk CdS which further confirms the formation of nanoparticles of CdS. The presence of well defined diffraction peaks in the XRD spectra, indicates formation of good crystalline structure in CdS sample. The average crystallite size of CdS nanoparticles was found to be 11.52 nm.

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