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Synthesis and Characterization of Cadmium Sulfide Nanoparticles

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Abstract

Cadmium sulfide nanoparticles were synthesized via chemical co-precipitation method from cadmium (II) chloride and sodium sulfide. The formed nanoparticle is characterized by powder x-ray diffraction, scanning electron microscopy, ultra-violet spectroscopy and fourier transform infrared spectroscopy, confirmed the preferential growth of cadmium sulfide nanoparticles that width is 31.54 nm. The SEM image shows the synthesized cadmium sulfide nanoparticles show well crystallized particles with irregular shape. The FTIR spectrum is used to study the stretching and bending frequencies of molecular functional groups in the sample. From UV spectrum, the band gap of cadmium sulfide nanoparticles is found to be 3 eV.

Keywords: XRD, SEM, FTIR, UV.

1. Introduction

CdS is a group II–VI semiconductor, and as such, CdS nanoparticles have generated great interest due to their unique size-dependent chemical and physical properties. Extensive research has focused on the synthesis of various CdS nanostructures. Cadmium sulfide occurs in nature as the mineral greenoktite. The compound is widely used in pigments for paints, baking enamels, ceramics and plastics. It imparts bright yellow to maroon, with strong retention of color and resistance to alkalis. It also is used in inks, phosphors, and fluorescent screens. Other applications of this compound are in photovoltaic and solar cells (for converting solar energy to electrical energy), photoconductors (in xerography), thin film transistors and diodes, rectifiers, scintillation counters, pyrotechnics, and smoke detectors. This paper deals with easy, simple, fast and low cost synthesis of cadmium sulfide nanoparticles by chemical co-precipitation method and its characterizations.

2. Materials and Methods

Nanoparticles of cadmium sulfide were prepared by chemical co precipitation method by adding cadmium (II) chloride and sodium sulfide. Precise amounts of reagents taking into account their purity were weighed and dissolved separately in distilled water into 0.1M concentration. After obtaining a homogeneous solution, the reagents were mixed using magnetic stirring. The precipitate was separated from the reaction mixture and washed several times with distilled water and ethanol. The wet precipitate was dried and thoroughly ground using agate mortar to obtain the samples in the form of fine powder [1].

3. Tests Conducted

X-ray diffraction is an ideal technique for the determination of crystallite size of the powder samples. The basic principle for such a determination involves precise quantification of the broadening of the peaks. XRD line broadening method of particle size estimation was chosen in this investigation for determining the crystallite size of the powder sample. The morphology of the powder samples was studied by the scanning electron microscope (SEM) analysis. The infra red spectroscopic (IR) studies of cadmium sulfide nanoparticles were made by using 'SHIMADZU' FTIR 8400S model spectrometer through KBr method. The UV spectrum was taken in the absorbance mode in the wavelength range from 200 to 800 nm.

4. Results and discussion

4.1. XRD studies

XRD – Particle Size Calculation

The XRD patterns of the prepared samples of cadmium sulfide nanoparticles are shown in figure.1. XRD studies reveal that the samples are nano sized and crystalline. The fine particle nature of the samples is reflected in the X-ray line broadening. The size of the synthesized cadmium sulfide nanoparticles are calculated using Scherrer equation(1)

$$D = 0.9\,\lambda / \beta \cos\theta \qquad (1)$$

where λ represents wavelength of X rays, β represents half width at full maximum and θ is the diffraction angle[2].

The average grain size of the particles is found to be 31.54 nm. The XRD pattern of cadmium sulfide nanoparticles is shown in figure 1.

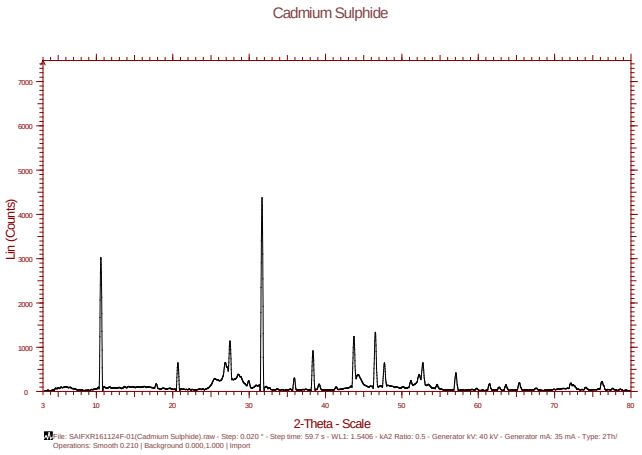

Figure .1. XRD pattern of cadmium sulfide nanoparticles.

A good agreement between the Experimental diffraction angle [2θ] and Standard diffraction angle [2θ] of specimen is confirming standard of the specimen. Many peaks at 2θ values of cadmium sulfide is observed and tabulated in table.1 and compared with the standard powder diffraction card of Joint Committee on Powder Diffraction Standards (JCPDS), cadmium sulfide file No. 02-0563.

Table.1. Experimental and standard diffraction angles of cadmium sulfide nanoparticles.

Experimental	Standard – JCPDS 02-0563
Diffraction angle (2θ in degrees)	Diffraction angle (2θ in degrees)
11.381	11.462
12.292	12.259
13.034	13.048
16.829	16.847
19.849	19.818
21.617	21.622
23.234	23.375
26.09	26.099
29.327	29.336
31.115	31.157
31.636	31.649
32.665	32.682
34.731	34.663
35.885	35.589
36.897	36.905
38.677	38.696
40.201	40.263
42.314	42.323
43.7	43.724
46.065	46.068
51.56	51.567

XRD – Dislocation Density

The dislocation density is defined as the length of dislocation lines per unit volume of the crystal. In materials science, a dislocation is a crystallographic defect, or irregularity, within a crystal structure. The presence of dislocations strongly influences many of the properties of materials. The movement of a dislocation is impeded by other dislocations present in the sample. Thus, a larger dislocation density implies a larger hardness.

The X-ray line profile analysis has been used to determine the dislocation density.

The dislocation density can be calculated from equation(2)

$$\delta = \frac{1}{D^2} \qquad (2)$$

Where δ is dislocation density and D is the crystallite size. Results of the dislocation density calculated from the formula is given in table.2. The number of unit cell is calculated from equation(3)

$$n = \pi\,(4/3) \times (D/2)^3 \times (1/V) \qquad (3)$$

Where D is the crystallite size and V is the cell volume of the sample.

Table .2. Dislocation Density and Number of Unit Cell from XRD of cadmium sulfide nanoparticles.

2θ (deg)	Particle Size D (nm)	Dislocation Density (m^2) x10^{15} $\delta = 1 / D^2$	Number of Unit Cell X10^5
10.492	31.16	1.029	1.268
20.596	32.04	0.974	4.111
31.635	31.54	1.005	1.644
43.699	31.29	1.021	1.605
46.506	29.98	1.113	1.412

It is observed from these tabulated details, and from figure.2, figure.3 and figure.4, dislocation density is indirectly proportional to particle size and number of unit cells. Dislocation density increases while both particle size and number of unit cell decreases.

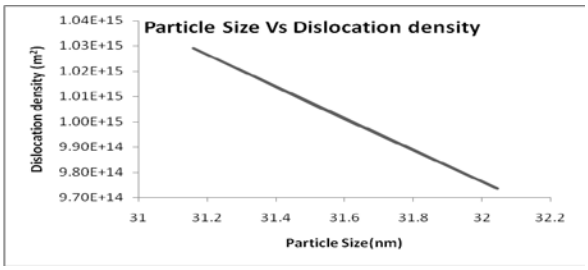

Figure.2. Particle size Vs Dislocation density curve of cadmium sulfide nanoparticles.

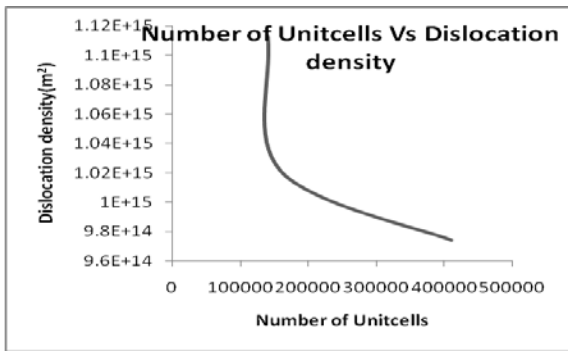

Figure.3. Number of Unit cells Vs Dislocation density curve of cadmium sulfide nanoparticles.

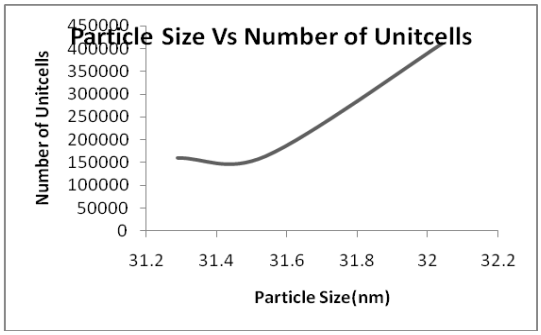

Figure.4. Particle Size Vs Number of Unit cells curve of cadmium sulfide nanoparticles.

XRD – Morphology Index

A XRD morphology index (MI) is calculated from FWHM of XRD data using the relation

$$M.I = \frac{FWHM_h}{FWHM_h + FWHM_p}$$

Where M.I. is morphology index, $FWHM_h$ is highest FWHM value obtained from peaks and $FWHM_p$ is value of particular peak's FWHM for which M.I. is to be calculated. The relation between morphology index and particle size is shown in table .3.

Table .3. Relation between Morphology Index and Particle size for cadmium sulfide nanoparticles.

FWHM (β) radians	Particle Size(D) nm	Morphology Index (unitless)
0.004506	30.79	0.5
0.004535	30.56	0.4984
0.004268	29.11	0.4362
0.004936	28.08	0.4772
0.005722	24.22	0.4405

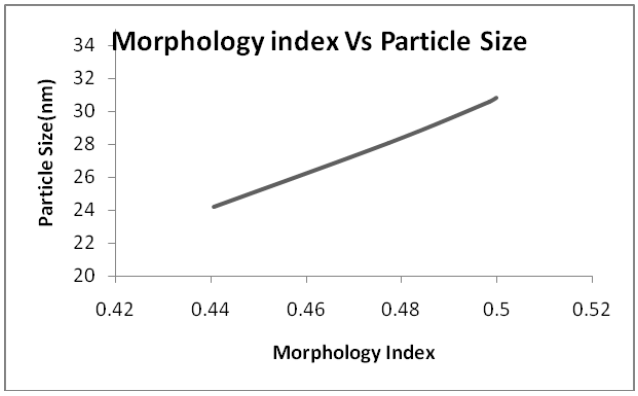

Figure .5. Morphology Index of cadmium sulfide nanoparticles.

It is observed that MI has direct relationship with particle size and the results are shown in Figure .5.

XRD – Unit Cell Parameters

Unit cell parameters values calculated from XRD are enumerated in table .4.

Table .4. XRD parameters of cadmium sulfide nanoparticles.

Parameters	Values
Structure	Hexagonal
Space group	P63mc (186)
Symmetry of lattice	Primitive
Particle size	31.54 nm
Lattice parameters	a=4.142;b=---;c=6.724
Vol.unit cell(V)	99.9
Density (ρ)	4.803
Dislocation Density	$1.054x10^{15}$
Mass	144.47amu

4.2. SEM studies

Scanning electron microscopy was used to analyze the morphology and size of the synthesized cadmium sulfide nanoparticles. Figure.6, Figure.7, Figure.8 and Figure.9 show the SEM images of the cadmium sulfide nanoparticles at various magnifications. The SEM images of cadmium sulfide nanoparticles show well crystallized particles with irregular shape. In this case the particles sizes are slightly increased and is also observed that the particles are distributed with agglomeration.

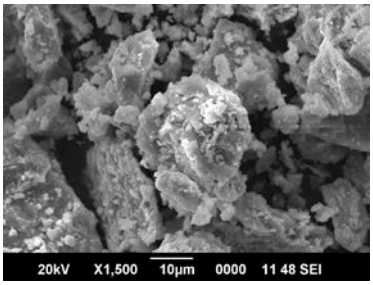

Figure.6. SEM image at 1500 magnifications.

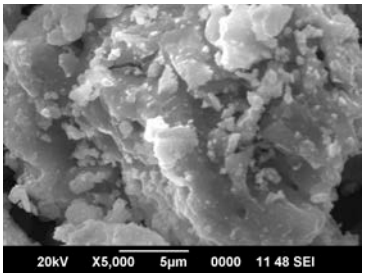

Figure.7. SEM image at 5000 magnifications.

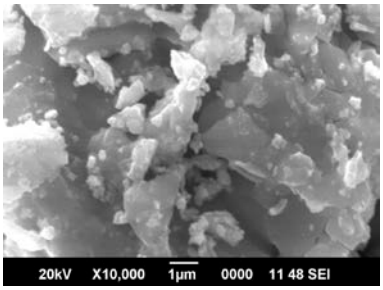

Figure.8. SEM image at 10000 magnifications.

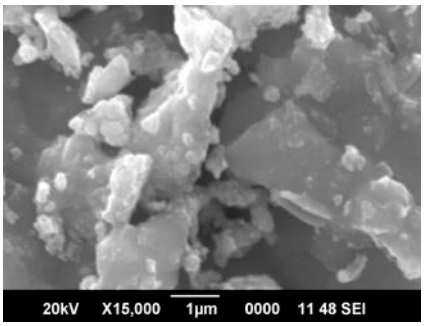

Figure.9. SEM image at 15000 magnifications.

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4.3. FTIR Studies

The FTIR spectrum of the cadmium sulfide nanoparticles is shown in the figure.10.The FTIR spectrum for cadmium sulfide nanoparticles show peak at 3519.07 cm^{-1}corresponds to the free O-H group and the peak at 1624.20 cm^{-1} is due to the presence of hydroxyl group of water and the peak at 1117.11 cm^{-1} corresponds to S-O bond and 616.57 cm^{-1} is due to S-S bond. The peak at 412.26 cm^{-1} responds to Cd-S bond [3].

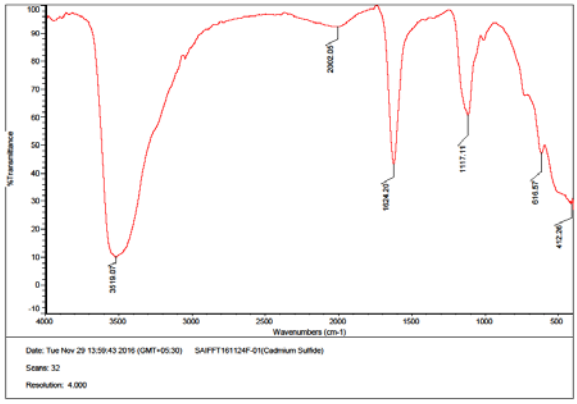

Figure.10. FTIR spectra of cadmium sulfide nanoparticles.

4.4. UV Studies

The band gap of the prepared sample cadmium sulfide nanoparticle was determined by using UV visible studies. Figure.11 shows the graph to find the band gap of cadmium sulfide nanoparticles. From the graph, the optical band gap of cadmium sulfide nanoparticles is 3eV.

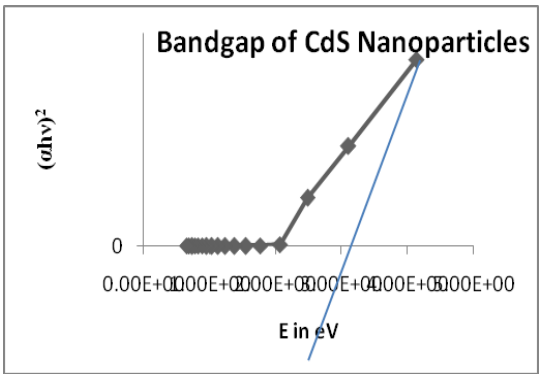

Figure.11. Graph to find the band gap of cadmium sulfide nanoparticles.

5. CONCLUSIONS

The cadmium sulfide nanoparticles have been prepared by chemical co-precipitation method. XRD analysis suggests that the average particle size is in the nano range (31.54nm). The SEM picture reveals the well crystallized particles with irregular morphology. From the FTIR spectrum, the stretching and bending frequencies of the molecular functional groups in the sample are studied. From the UV spectra, the band gap was found.

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