SYNTHESIS AND CHARACTERIZATION OF CdS NANOPARTICLES FOR NANO ELECTRONIC DEVICE APPLICATION

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Abstract
The chemical co-precipitation approach was used to make cadmium sulfide (CdS) nanoparticles in this study. The produced samples' structural, elemental composition, and morphological features were investigated. Cadmium and sulfur were obtained from cadmium chloride and thiourea. The X-ray diffraction (XRD) technique was used to determine the crystalline structure, crystal size, interplaner space, lattice parameter, unit cell volume, and microstrain caused in the lattice. At room temperature, XRD results reveal CdS hexagonal Wurtzite (WZ) structural phases. The average grain size was discovered to be in the nanometer range, confirming the existence of nanoparticles. The nanoparticles have a smooth surface and appear to be generally spherical in shape, according to FESEM micrographs, with a crystallite size of 12.76 nm. Cadmium (Cd) and Sulfur (S) are present in almost stoichiometric proportions, according to EDAX analysis. CdS are suited for optoelectronic device applications, according to the research.

Keywords: Cadmium sulfide, Nanoparticles, Nanoelectronics device.
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Introduction

Nanomaterials have attracted people's curiosity because of their unique structural and optical properties that set them apart from bulk solids and molecules. Because innovative features of nanomaterials are determined by their size, structure, and form, a better knowledge of the mechanisms by which these properties might change, as well as a new approach for synthesis processes, could be important challenges in nanoscience. The surface characteristics of nanoparticles have a major influence on their structure and, as a result, on their nanoscale devices in a variety of technological domains, from electronics to targeted pharmaceuticals. This is due to the high surface-to-volume ratio of nanoparticles. The removal of surface imperfections from nanoparticles by modifying their surfaces with various organic or inorganic species is expected to alter their characteristics. Surfactant-coated nanoparticles would provide an aggregation barrier and electrical passivation [1].

The Binary compounds PbS, ZnS, ZnSe, CdS, CdSe, CdTe, Ternary compounds GaAsP, AlGaAs, etc, and quaternary compounds like In GaAsP, etc. are the Semiconducting materials generally used in electronic and optoelectronic devices [2]. The II-VI binary compound CdS is the most promising choice among the above-mentioned compounds due to its spectrum response in the UV-Visible range and its ability to absorb electromagnetic waves (visible light, UV, & IR), CdS is employed as window material in various optoelectronic devices.

When a semiconductor absorbs light, the number of free electrons and electron-hole pairs increases, increasing its electrical conductivity. The light that reaches the semiconducting materials must have enough energy to raise electrons across the bandgap in order for this to happen. The bandgap is a critical characteristic of semiconductors. Infrared photodetectors and thermoelectricity both require narrow bandgap materials whereas Light-emitting diodes [3], solar cells [4], and other devices use materials with a greater bandgap.

Crystallization, sol-gel, chemical vapor deposition, spray pyrolysis [5], and other procedures for the formation of nanoparticles are some of the methods for the production of CdS. We used a low-cost chemical co-precipitation approach to produce cadmium sulfide (CdS).

Experimental Details

Synthesis

All the chemicals and reagents of analytic grade (A.R) were used. In this synthesis precursors, cadmium chloride dihydrate ($CdCl_2$. H_2O, 99.99 %), Thiourea ($CS(NH_2)_2$, 99.99%) were used as the source of Cd and S respectively. An aqueous solution of NaOH (0.2 M) is used for suitably adjusting PH value. The deionized water was used as a solvent for the preparation of solutions. An aqueous solution of $CdCl_2$ (0.1M) and Thiourea (0.1 M) were prepared and mixed stoichiometrically. The solution was stirred continuously at room temperature for 30 minutes then another prepared solution of NaOH (0.2M) was added dropwise with the above solution and stirred magnetically. After some time, a clear homogeneous yellow-colored colloidal solution was obtained and kept for 24 hours. The yellow-colored precipitate obtained at the bottom of the vessel was filtered and washed several times. The filtrate was dried in presence of IR at 90^o C for 8 hours and crushed into fine powders and then finally annealed at 200^oC in a muffle furnace for the removal of volatile impurities.

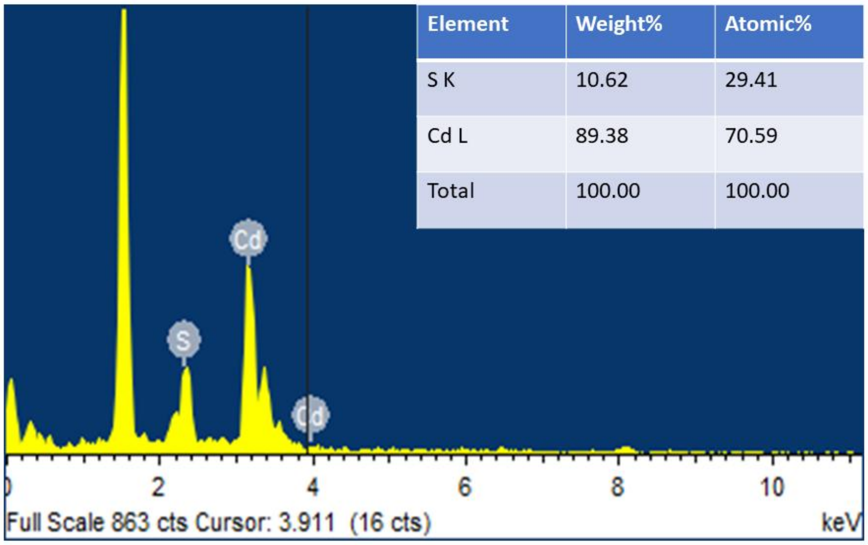
Characterization

X-ray diffraction is used to determine the structure and phase of the sample using a Rigaku X-ray diffractometer (PANalytical X'Pert Pro) and CuKα radiation. The sample's surface morphology was investigated using a scanning electron microscope (SEM) and Energy Dispersive X-ray spectroscopy (EDX).

Results and Discussion

Elemental Analysis:

The EDAX technique is used to determine the presence of quantitative elemental composition of the prepared CdS nanoparticles. Fig (1) shows the EDAX spectra of CdS nanoparticles, which clearly reflect the presence of cadmium (Cd) and sulfur (S) and the absence of other impurities or contaminants in the samples.



Element	Weight%	Atomic%
S K	10.62	29.41
Cd L	89.38	70.59
Total	100.00	100.00

Fig. 1. EDAX Spectra of CdS nanoparticles.

Surface Morphology:

The morphology of CdS nanoparticles has been investigated by FESEM at 10,000X magnification, the scale bar length is 1 micrometer and the average grain size was estimated. Fig. (2) and Fig. (3) show the image of FESEM micrographs of the CdS nanoparticles. The micrograph clearly indicates that the nanoparticles have a smooth surface and appear to be roughly spherical. The particles are found to be agglomerated, which might be due to the absence of a capping agent in the prepared solution during synthesis. The average grain size obtained from FESEM images is found to be in the nm range.

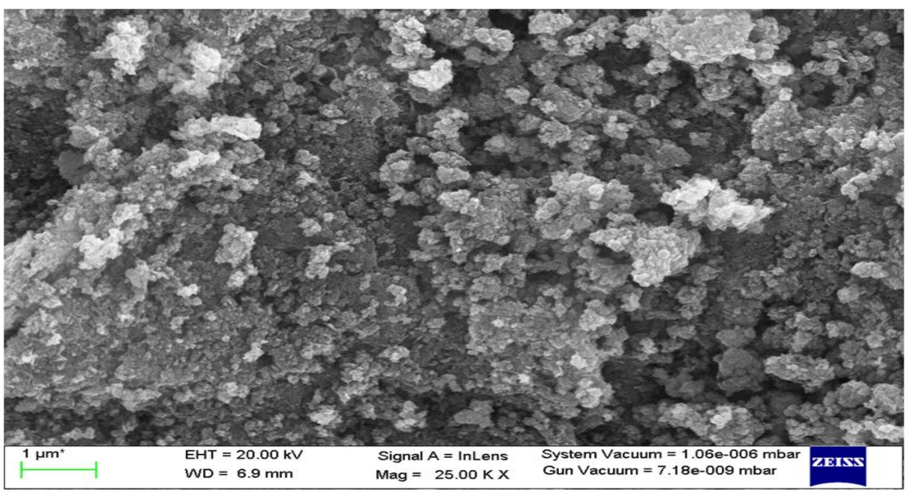


Fig. 2. FESEM image of CdS.

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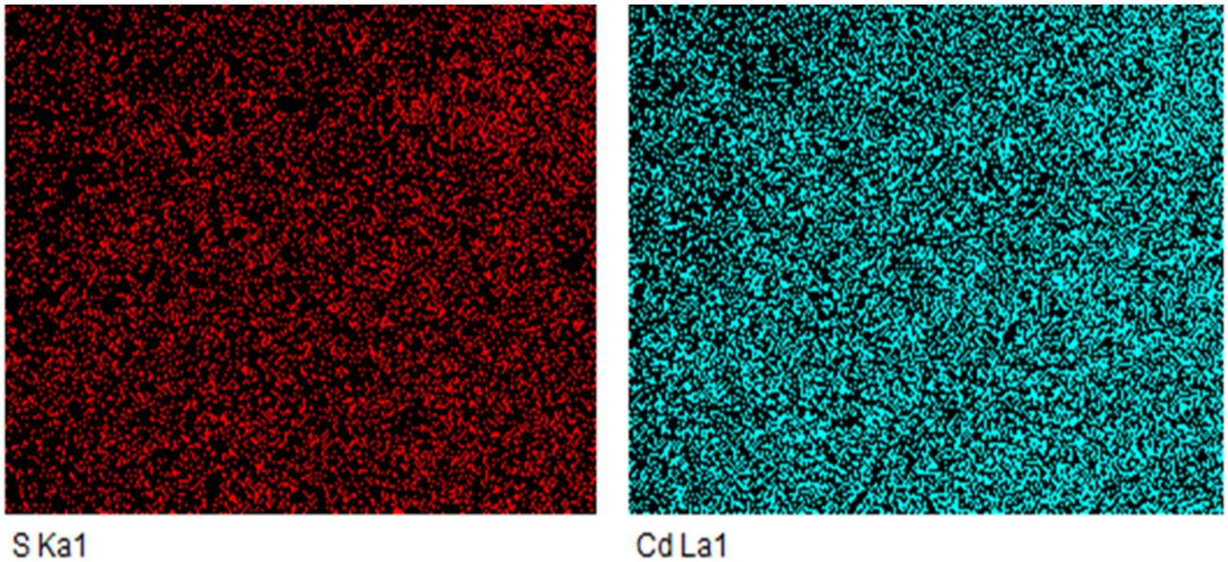

Fig. 3. Mapping image of Cadmium and Sulfur.

Structural Analysis:

Structural analysis was carried out by XRD-Technique. XRD diffraction spectra shown in fig. (4) have been recorded using Cu-kα radiation of wavelength (λ=1.5406 Å) in the range of angle 20 to 65 degrees to determine the crystal structure.

All the major peaks in the diffraction spectra of CdS observed at angles of 25.15, 26.84, 29.61, 37.64, 44.24, and 52.22 correspondings to the planes (100), (002), (101), (102), (103), and (112) respectively. The standard diffraction peaks show the hexagonal wurtzite structure of CdS NCs with the $P6_{3\ mc}$ space group and are also verified by the JCPDS card number 10-0454[6]. The broadening of the peaks supports the formation of nanocrystals.

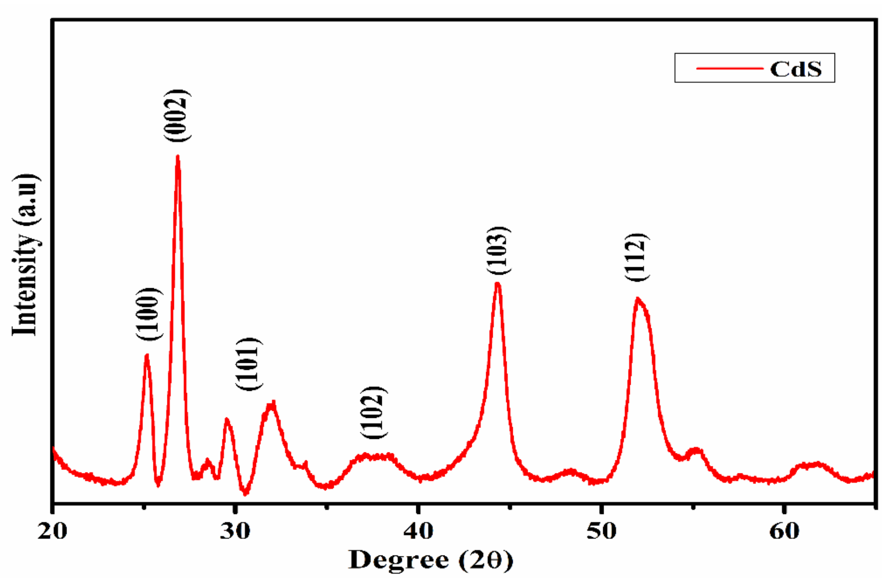

Fig. 4. XRD Spectra of CdS.

The crystallite size of the samples was calculated at the FWHM of the peak of the plane (002) using Debye-Scherrer's formula [7]:

$$D = \frac{0.9\lambda}{\beta cos\ \theta}$$

Where D is the crystallite size.

λ is the wavelength of X-ray radiation (1.54060 Å) and

β is the full-width half maxima (FWHM) and θ is the diffraction angle.

The interplanar space has been estimated using Bragg's law:

$$n\lambda = 2d\sin\theta$$

Where n (=1) is the order of diffraction

λ is the wavelength (1.54064Å) of the X-ray used

θ is the diffraction angle and 'd' is the interplanar space

and then the equation:

$$\frac{1}{d^2} = \frac{4}{3}\left(\frac{h^2 + hk + k^2}{a^2}\right) + \frac{l^2}{c^2}$$

Where, 'd' is the inter planer space

(h, k, l) are the Miller indices and

'a' and 'c's are the lattice constants of the unit cell.

The lattice constant 'a' is obtained for the plane (100), through the relation

$$a = \frac{\lambda}{\sqrt{3}\ Sin\ \theta}$$

The lattice constant 'c' is derived for the plane (002) by the relation

$$c = \frac{\lambda}{Sine\ \theta}$$

The volume of the unit cell is calculated from the value of the lattice constants by using the relation:

$$V = \frac{\sqrt{3}}{2}a^2 c$$

Estimation of elastic parameters:

The microstrain present in the nanoparticles and deformation are calculated using the following expression [9]:

$$\epsilon = \frac{\beta}{4 \tan \theta}$$

The estimated value of ε for CdS is found at 0.01806 µm/m.

The dislocation density, which defines the length of dislocation lines per unit volume of crystal of the nanoparticles, which is used to analyze the disorders, deformation, irregularities, and crystal defects present in samples, can be calculated using the following expression [10]:

$$\delta = \frac{1}{D^2}$$

The estimated values of δ for CdS nanoparticles is found at 1.88 lines/meter.

Table 1-The calculated values of crystallite size, interplanar space, lattice constants, and volume of the unit cell.

Sample	Peak position '2θ' (Degree)	Plane (hkl)	FWHM (Degree)	Inter-planar spacing d (Å)	Crystallite size D (nm)	Lattice constants		c/a	Volume of the unit cell 'V' ($Å^3$)
						'a'(Å)	'c' (Å)		
CdS	26.8405	(002)	0.0095	3.5379	12.7631	4.0853	7.0758	7.0758	102.2741

Conclusion:

The X-ray diffraction (XRD) technique is used to know the structural behavior of prepared CdS nanoparticles, crystallite size, lattice parameters, strain, and dislocation densities have been estimated. The XRD spectra confirm the formation of the hexagonal (wurtzite) structural phase of CdS NPs. The boarding in the XRD peaks indicates the very small size of the NPs. The crystallite size corresponding to the plane (002) of the most intense peak is found 12.76 nm. The structural investigation of CdS revealed that this kind of NPs can play an important role in the fabrication of nanoelectronics devices.

References:

[1] De Souza, Carla Daruich, Beatriz Ribeiro Nogueira, and Maria Elisa CM Rostelato. "Review of the methodologies used in the synthesis gold nanoparticles by chemical reduction." *Journal of Alloys and Compounds* 798 (2019): 714-740.

[2] Gupta, K. M., and Nishu Gupta. "Semiconductor materials: their properties, applications, and recent advances." *Advanced Semiconducting Materials and Devices*. Springer, Cham, 2016. 3-40.

[3] Rodríguez-Mas, Fernando, et al. "Expanded electroluminescence in high load CdS nanocrystals PVK-based LEDs." *Nanomaterials* 9.9 (2019): 1212.

[4] Martínez-Alonso, Claudia, et al. "Solution synthesized CdS nanoparticles for hybrid solar cell applications." *Journal of Materials Science: Materials in Electronics* 26.8 (2015): 5539-5545.

[5] Ilican, S., Y. Caglar, and M. Caglar. "Preparation and characterization of ZnO thin films deposited by sol-gel spin coating method." *Journal of optoelectronics and advanced materials* 10.10 (2008): 2578-2583.

[6] Elilarassi, R., S. Maheshwari, and G. Chandrasekaran. "Structural and optical characterization of CdS nanoparticles synthesized using a simple chemical reaction route." *Optoelectron. Adv. Mater* 4 (2010): 309-312.

[7] Patra, Prashanta, et al. "Structural, morphological, and optical properties of CdS and nickel doped CdS nanocrystals synthesized via a bottom-up approach." *Materials Today: Proceedings* 56 (2022): 811-818.

[8] AlkhayattOmran, AdelH, and Mohammad Rassol Ahmed. "Impact of reaction temperature on the structural, surface morphology and antibacterial activity of hydrothermally synthesized CdS nanoparticles." *Journal of Physics: Conference Series*. Vol. 1879. No. 3. IOP Publishing, 2021.

[9] Patra, Prashanta, et al. "Ni-incorporated cadmium sulphide quantum dots for solar cell: An evolution to microstructural and linear-nonlinear optical properties." *Journal of Crystal Growth* (2022): 126542.

[10] Sankar, M., et al. "Structural, optical and Photocatalytic degradation of organic dyes by sol gel prepared Ni doped CdS nanoparticles." *Surfaces and Interfaces* 21 (2020): 100775.

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