International Journal For Technological Research In Engineering
Volume 4, Issue 11, July-2017 *ISSN (Online): 2347 - 4718*

SYNTHESIS AND CRYSTALLOGRAPHIC STUDY OF CHROMIUM DOPED ZINC SULPHIDE NANOPARTICLES

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Abstract: Sample nanoparticles were synthesized by chemical co-precipitation route at normal temperature. In which chromium (III) nitrate (Cr (NO3)3.9H2O) is used as doping agent. Two samples of desired concentration i.e. 0.5M and 1M are synthesized. The size of the particle is controlled by using poly (vinyl alcohol) (PVA) which is added drop wise during sterrering process along with chromium nitrate solution. Obtained precipitate is washed, dried and crushed to obtain powdered sample. The XRD pattern shows that the given sample nanoparticle has cubic structure.

It is observed that on increasing the concentration of doping agent, nucleation and growth of the particle increases which increases the particle size, result in decrease in band gap. The obtained crystal size is 31.1nm. Decrease in Band gap can be seen clearly on increasing the Chromium concentration i.e. from 3.86 to 3.25eV. UV-Visible spectroscopy examine that the given sample have absorbance towards blue shift from (250nm-350nm) of wavelength. The functional group is determined and also the structure of molecule and arrangement of atoms are determined by observing various electronic transitions.
Keywords- Co precipitation, Poly (vinyl alcohol), electronic transition, Band gap, functional group, nucleation and growth, XRD, UV-visible spectroscopy.

I. INTRODUCTION

There are various chemical based methods available for the synthesis of Cr: ZnS nanomaterials. The purpose of the present work is to synthesize Cr: ZnS nanoparticles using chemical Co precipitation method and to investigate the structural and optical properties using XRD, and ultraviolet visible spectroscopy. All these interesting properties of Cr: ZnS like electrical, optical, physical and chemical properties of the material are determined. Among all semiconductor nanoparticles, zinc sulphide (ZnS) is an interesting material with many applications in various fields such as optoelectronics, photo catalysis, solar energy conversion, projection television, fluorescence microscopy, etc.

Nano-sized semiconducting materials have been generating an extensive interest in recent years owing to their structural, chemical and physical properties which are different from those of the bulk materials. These improved physical properties can be ascribed to the various phenomena like quantum confinement of electrons, surface disorder etc., that takes place in the nano-regime. The quantum confinement of excitons in semiconductor nanostructures can cause widening of the band gap, thereby making them eligible for optoelectronic applications. The surface of nano-particles are highly disordered which is the reason behind the huge value of electrical conductivity they exhibit [1]. Hence a detailed investigation in to the underlying reasons of novel properties that nanomaterials possess would be in the interest of the world. ZnS has wide band gap of 3.91 eV and the band gap energy can be tuned in the UV region.

It is an important material for a variety of applications including photoconductors, solar cells, and field effect transistors, sensors, transducers, optical coatings and light emitting materials. In this paper we have synthesize one of the doped nanoparticles i.e. Cr: ZnS by chemical co precipitation route.

II. EXPERIMENTAL

Cr doped ZnS with chemical composition Zn1-xCrxS (x = 0.5% and 1%) were synthesized by chemical co precipitation route. All chemicals were used of analytical grade. Distilled water was used as solvent. The starting materials Chromium doped ZnS nanocrystals with pure and 10% compositions were synthesized by chemical co-precipitation route zinc Chloride, chromium nitrate and sodium sulfide. The appropriate amounts of zinc Chloride and chromium nitrate were dissolved separately in 100 ml distilled water and stirred at room temperature for 2 h. Chromium nitrate solution was added into zinc nitrate and stirred for 20 min.

A high alkaline medium (pH-10) was maintained by adding sodium sulphide solution into mixed solution of zinc nitrate and chromium nitrate drop wise, the light sky-blue coloured precipitate was obtained, the colour of the precipitate becomes dark on increasing the concentration by 10%. Then the solution is filtered and dried at 60 0C, samples of Cr: ZnS are obtained [2]. The precipitate was collected and washed several times by DI water and methanol. Finally to get pure Cr doped ZnS nanocystals, the precipitate was dried in the oven at 50 oC for 4 h.

The X-ray diffraction patterns of 0.5M doped and 1M Cr doped ZnS nanocrystals were recorded using XRD radiation (Bruker, λ=1.5406 Å) with 2θ ranging 0-80o. The UV-Vis measurements were done with UV-Vis spectrometer (Jasco UV-VIS-NIR spectrophotometer V-670) in the wavelength range of 200 nm to 1000 nm.

The flow chart for synthesis process is described in the fig.1. given below:-

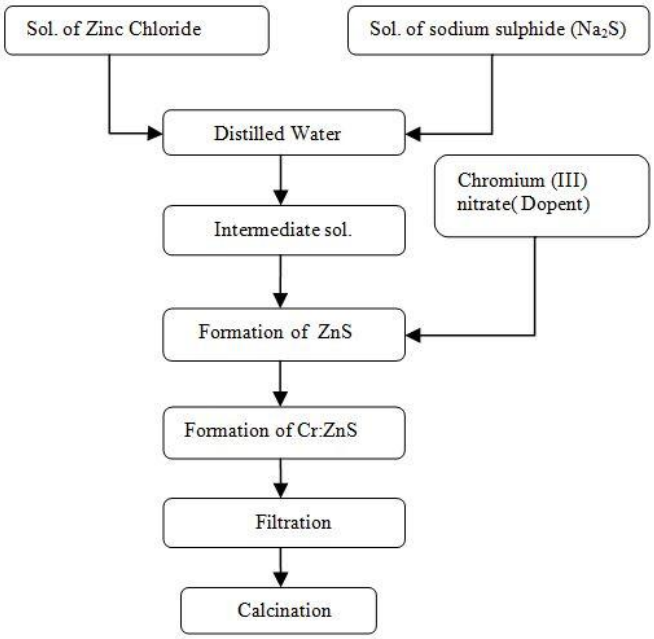

Fig.1 The flow chart of preparation Cr: ZnS nanoparticles by chemical co-precipitation method.

Crystallographic study

Structural Characterization: - The X-ray diffraction (XRD) patterns of Cr:ZnS nanoparticles were recorded by Bruker system using radiation (λ=1.54184 nm) with 2θ ranging 0–80° and the value of d=3.08029.

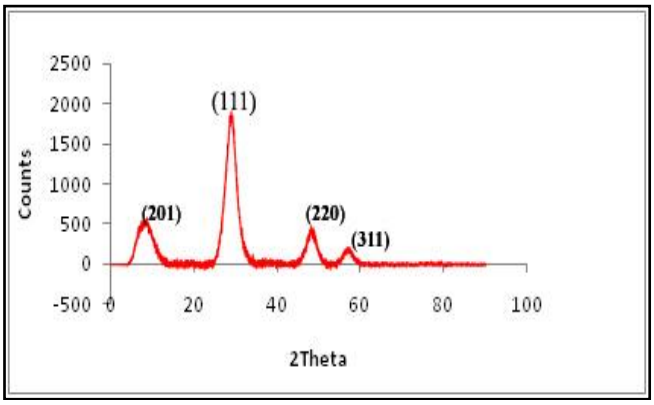

Fig. 2 XRD patterns of Cr:ZnS nanoparticles.

The X-ray diffraction (XRD) patterns of ZnS nanoparticles were recorded by Bruker system using radiation (λ=0. 1.54184 nm) with 2θ ranging 0–80°. The nanoparticles size was also estimated using the Scherrer formula (Scherrer 1918) from the XRD data as above,

$$t = \frac{k\lambda}{B\cos\theta}$$

Where,

t= mean size of ordered crystals.

B = Full Width at Half Maximum (FWHM=2.936).

K=Shape function.(K=1)

λ= X- Ray wavelength (i.e. 1.54184)

θ = Brag's angle. (θ=28.738)

Gross intensity=12.

Net height= 11.7.

Crystal size= 31.1nm.

Where λ, B, and θ are the X-ray wavelength of the radiation used the full width at half maximum (FWHM) of the diffraction peak and the Bragg diffraction angle, respectively. The structure of nanoparticles is found to be cubic by the data analysis of XRD [3].

XRD patterns of Cr doped ZnS nanocrystals are as shown in Fig 2. The broadening of diffraction confirmed that the crystallites were nanosized. The diffraction peaks corresponds to (201), (111), (220) and (311) planes are in good agreement with the standard diffraction peaks (JCPDS 00-001-0792) of cubic structure and also indicates that the Cr^{2+} ions substituted into Zn^{2+} site has no effect on the crystal structure. No additional peaks were observed. The lattice parameter, volume cell, X-ray density, grain size and % of crystallinity were determined using XRD data. Grain size of the nanoparticles determined by the Debye-Scherrer's equation is 31.1nm. Cr doped ZnS nanocystals synthesized by co-precipitation route was wurtzite cubic structure. In the present investigation the (111) diffraction peak is also shifted to higher angle for 10% Cr doped ZnS in comparison to pure ZnS samples. It may be due to the small ionic radii of Cr^{3+} (0.63 Å) compared to that of Zn^{2+} (0.74 Å), which have entered into the lattice site of ZnS. Our XRD data is in good agreement with the diffraction data of cubical structure and the cell parameter 'a' is very close to the reported value in JCPDS 00-001-0792 data [4]. From attribute that the grain size and the X-ray density are more and lattice parameter 'a', volume of unit cell and % of crystallinity are less for 1M Cr doped ZnS than in 0.5M doped nanocystals.

III. UV-VISIBLE SPECTROSCOPY

The absorption edge is observed in the range of 200–300 nm, which is blue shifted compared to bulk ZnS. As the Cr concentration increases, the absorption edge shifts to lower wavelength side and intensity also increases with increasing Cr concentration compared to undoped ZnS. This blue shift of the absorption edges for different sized nanocrystals is related to the size decrease of particles and is attributed to the quantum confinement limit reaching of nanoparticles. The quantum confinement effect is expected for semiconducting nanoparticles, and the absorption edge will be shifted to a higher energy when the particle size decreases Absorption coefficient (α) of the powders at different wavelengths can be calculated from the absorption spectra.

The absorption spectra for the two samples (0.5M and 1M) is shown in Fig. 3

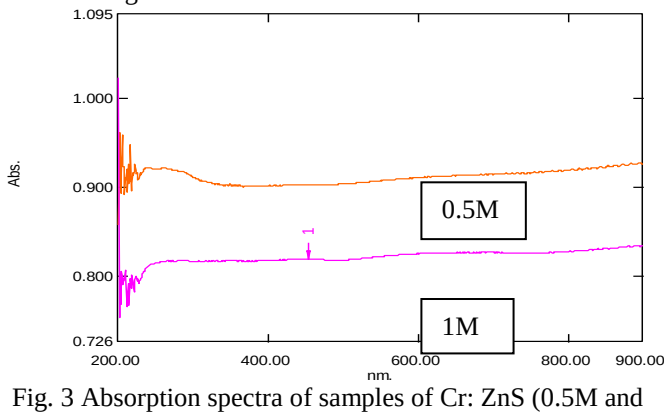

Fig. 3 Absorption spectra of samples of Cr: ZnS (0.5M and 1M) nanoparticles.

CrxZn1-xS (x=0-0.1)	Energy band gap (Eg) eV
ZnS	3.91
Cr:ZnS(0.5M)	3.86
Cr:ZnS(1M)	3.25

Table 2 Showing band gap comparison of pure ZnS with Cr impurity doped ZnS.

IV. RESULT AND DISCUSSION

It is possible to produce different size Cr: ZnS nanoparticles using a simple chemical co precipitation method with using different molar concentration of capping agent. XRD confirm nano-size of these particles having cubic structure. It is also observed that the particle size depends on molar concentration of capping agent. A decrease in formation rate of nanoparticles gives rise to a larger final particle size for all the synthesis conditions. As the particle size depends on the molar concentration of doping agent, a decrease in the size of particle is observed with the increase of molar concentration of capping agent. The mean crystallite size range of particles was between 2.24 and 35.43 nm, depending on molar concentration of capping agent. The values UV-Visible exhibit a blue shift which is related to the size decrease of the particles and to the quantum confinement limit reaching of nanoparticles [5]. Considering these results, the chemical co-precipitation method using, Poly (vinyl alcohol), as a capping agent is very efficient for the preparation of Cr: ZnS nanoparticles in order to control the particle size and also for modern optoelectronic applications. The gain material is susceptible to utilization of direct diode or fibre laser pumping of a microchip laser with a level of power density providing formation of positive lens and corresponding cavity stabilization as well as threshold population inversion in the laser material. It also has many applications in various fields such as optoelectronics, photo catalysis, solar energy conversion, projection television, fluorescence microscopy, etc. Multiple applications of the material are contemplated in the invention.

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