Research Journal of Chemical Sciences _____ ISSN 2231-606X
Vol. **2(8),** 69-71, August **(2012)** *Res.J.Chem.Sci.*

Short Communication

"Green" Synthesis of CdS nanoparticles and effect of capping agent concentration on crystallite size

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Available online at: www.isca.in
Received 15th April 2012, revised 19th April 2012, accepted 20th April 2012

Abstract

In recent years, the synthesis of CdS nanoparticle has attained great attention due to its unique size dependent optical, catalytical and electrical properties. CdS nanoparticles are II-VI group semiconductor in nature with a wide band gap. Simple, non toxic and environmental friendly method of its production has been described here using glucose as passivator. Characterization has been done by using (XRD) X-Ray Diffraction and UV Visible Spectroscopy.

Keywords: Green synthesis, Nanoparticles, XRD, UV Visible Spectroscopy

Introduction

Integration of principles of "Green Chemistry" in Nanosciences has attracted researchers in recent years. Simple and novel method of semiconductor nanoparticle synthesis is now a great area of interest. Semiconductor nanoparticles show size dependent luminescence, optical and electrical properties which find a number of applications in many areas[1,2]. CdS nanoparticle belongs to the group of Chalcogenides is a II-IV group semiconductor nanoparticle and shows size dependent properties due to its very high surface to volume ratio and quantum confinement at nanoscale. CdS nanoparticles also have very high photosensitivity that makes them a promising candidate for the detection of visible radiations, enhancing efficiency of solar cells, in LEDs, as sample photoconductor in optoelectronic devices[3] and a number of biological applications[4]. The energy band gap goes on increasing with a decrease in size[5, 6]. Due to these unique properties plants are now being established for its large scale production. The commonly used capping agents for its synthesis such as mercaptoaccetate, thiourea, thiophenol etc., are toxic in nature and their large scale production poses a potential threat to the environment[7, 8]. Thus, here we are describing a simple and novel method for the synthesis of CdS nanoparticle by using glucose as capping agent and studying the effect of capping agent concentration on crystallite size. UV visible spectrum is recorded for studying blue shift and increase in the band gap.

Material and Methods

Synthesis of CdS nanoparticle: Chemicals and reagents used in the present study were of analytical grade (>99%) and used without further purification. A simple chemical route was followed for the synthesis of CdS nanoparticles[9]. Cadmium nitrate was utilized as a source of cadmium ions and as sulfide source sodium sulfide was used. Glucose was used as capping agent. Synthesis can be summarized in the equation given below:

$$Cd(NO_3)_2 + Na_2S \xrightarrow{\text{Glucose}} CdS + NaNO_3$$

In cadmium nitrate solution (0.1 M), sodium sulfide (0.1 M) was added drop wise with continuous stirring. A pale yellow colored solution was formed which was further shaken on a magnetic stirrer for 15 hours. The solution was divided into three parts and 10 ml of 0.01M, 0.1M, 0.5 M glucose solution was added drop wise in each part of the solution respectively. The samples were heated and incubated at 100^0C for more than 6 hours. Precipitates were filtered and dried at 50^0C for 4 hours for decreasing its very high surface energy to avoid cluster formation of nanoparticles.

Characterization of CdS nanoparticle: X Ray Diffraction was performed by using Rigaku Miniflex X ray diffractometer which utilized CuKα (1.54 Å) as target material[10]. XRD data were used to determine the lattice parameter, crystallite size and phase identification.

Crystallite size was calculated by applying Sherrer's equation[11].

$$d = 0.9\lambda / \beta \cos\theta$$

Where, d is the crystalline size, λ is the wavelength of the CuKα (1.54 A°), θ is the angle between the incident beam and the reflecting lattice plane and β is the full width at half maxima (FWHM) of the diffraction peak (in radian).

Lattice constant was calculated by applying the formula:

$$a = d\,(h^2+k^2+l^2)^{1/2}$$

Where, a is lattice constant, d is interplanar spacing and h, k, l are lattice planes. Interplanar spacing was calculated by applying the formula:

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

Where, θ is the angle between the incident beam and the reflection lattice planes and λ is the wavelength of the CuKα (1.54 Aº).

The absorption spectrum was recorded by using Camspec M550 Double Beam Scanning UV Visible spectrophotometer and the energy band gap was calculated by employing direct formula[12]:
Eg^0 (eV) = 12397.8 / λ_{max} (Å)

Where, Eg^0 is an energy band gap and λ_{max} is the wavelength at which maximum absorption was shown.

Results and Discussion

Structural characterization of CdS nanoparticle: Synthesis and crystallite size of nanoparticles were significantly influenced by the concentration of capping agent. It was found that the crystallite size decreased from 43-13 nm as the concentration of capping agent (glucose) increased from 0.01, 0.1 and 0.5 M, figure-1.

The XRD data for three samples having different concentrations of capping agents has been shown in figure-2. The presence of two peaks at 27.4, 47.5 confirmed the presence of cubic phase of CdS nanoparticles according to JCPDS file no. 10-454 corresponding to (111) and (220) planes respectively. It was observed that broadening in peaks at high concentration of glucose occur due to decrease in crystallite size. The shoulders in the (111) diffraction peaks may result from the X-ray irradiation on the sample as the cubic CdS are a metastable phase[13]. X-ray irradiation may induce a phase transition from cubic phase to hexagonal phase of CdS to some extent resulting in the appearance of the shoulders. Lattice constant comes out to be 5.75 Å for (111) plane and 5.43 Å for (220) plane. The results depicts that (111) plane has high intensity; therefore 5.75 Å considered as lattice constant, figure- 2.

Further, characterization was confirmed by measuring the optical Properties of CdS nanoparticle. An absorption spectrum was obtained by UV Visible spectroscopy in the range of 200 - 600 nm. The absorption spectrum was shown λ_{max} at 470 nm by 13 nm nanoparticle that confirmed a blue shift of about 45 nm as compared to bulk whose λ_{max} 515 nm[14,15], figure-3.

This blue shift effect arises due to quantum confinement. The direct energy band gap comes out to be 3.69 eV for 13 nm nanoparticle. The increase in band gap of 0.27 eV as compared to bulk 2.42 eV was due to size effect[16].

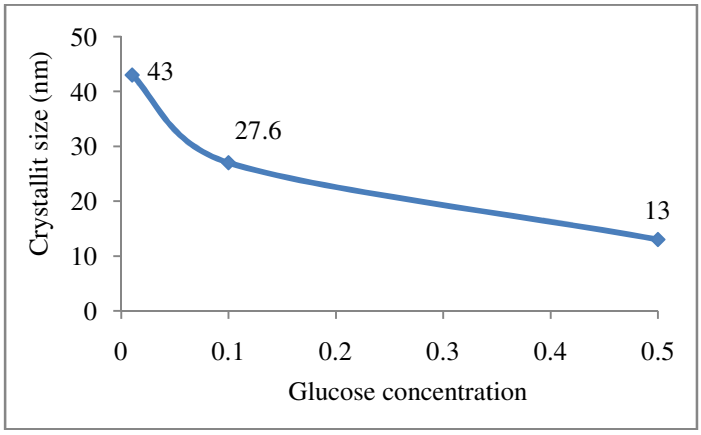
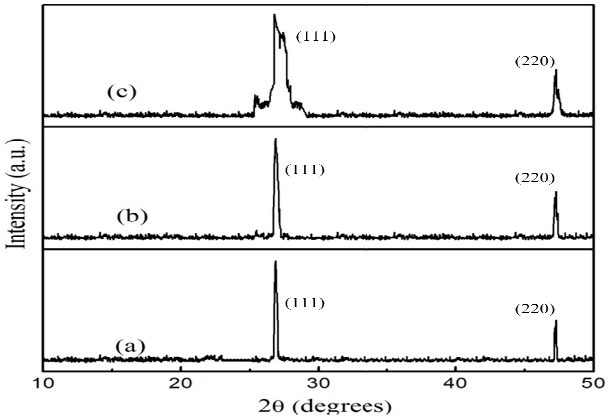


Figure- 1
Effect of glucose concentration on crystallite size of nanoparticle



Figures- 2
XRD data for crystallite size (a) 43 nm, (b) 27.6 nm, (c) 13 nm

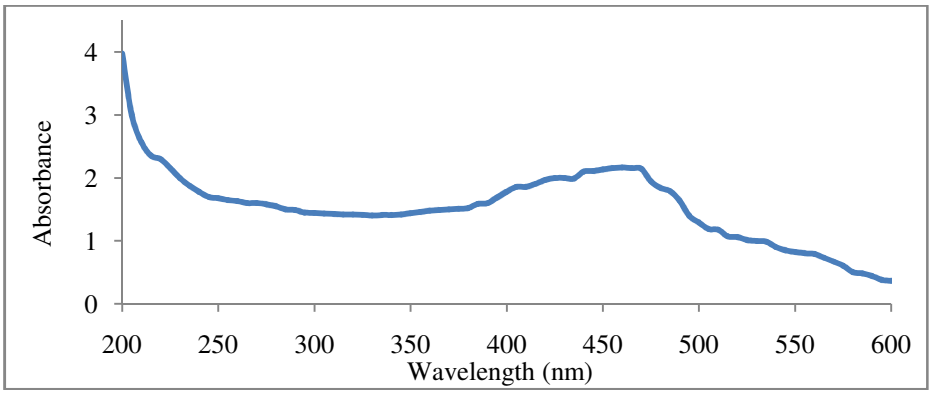


Figure- 3
UV Visible spectrum for 13 nm CdS nanoparticle

Conclusion

A simple Chemical colloidal method of CdS nanoparticle synthesis was developed by using glucose as capping agent. This method is eco-friendly for commercial scale production as it does not involve the use of hazardous and toxic capping agents such as thiophenol, thiourea and mercaptoaccetate. Further, capping agent concentration had significant effect can be seen in crystallite size and a blue shift was seen in $\lambda_{max.}$

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