Structural, Morphological and Optical Properties of CdSe(S) Quantum Dots

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Abstract. Semiconductor nanomaterials are tiny light emitting particles and have stimulated great interest among researchers might be due to their applications in solar energy conversion, optoelectronic devices, molecular and cellular imaging and ultrasensitive detection. The present study reports a facile and low-cost synthesis strategy of CdSe(S) nanoparticles via chemical co-precipitation method by controlling the experimental protocols. FTIR spectral study confirms the presence of CdSe(S) nanoparticles. XRD spectra suggest for their polycrystalline nature and prominent peak corresponding to cubic structure of CdSe(S) quantum dots. Besides this, some peaks corresponding to other structures, such as hexagonal, are also present. The crystallite sizes of grown CdSe(S) quantum dots were found to be 3 nm, 5 nm and 6 nm, respectively. The particle size obtained by TEM analysis was also in the range of 3nm to 8nm which agrees well with those reported by the XRD data. Low value of energy band gap shows their polycrystalline nature. Moreover, the as prepared CdSe(S) were found to exhibit quantum confinement effect, which leads to spatial enclosure of electronic charge carriers within the nanocrystals.

Keywords: Quantun Dots, Cadmium Selenium Sulphide, XRD, FTIR, TEM, Nanomaterials, Nanoparticles, Semiconductor.

INTRODUCTION

Quantum dots(QD) is semiconductor nanostructure that confines the motion of conduction band electrons, valence band holes or excitons in all the three spatial directions. The QDs were reported in 1980s by Alexei Eleimov in a glass matrix and by Burs in colloidal solutions. The QDs have been studied extensively, because of their unique, size dependent optical, electronic and magnetic properties, size tunable luminescence, narrow photoluminescence band and broad absorption spectra. Chemically synthesized nanoparticles have an advantage over physically prepared nanoparticles because they can be easily tailored to different shapes and sizes [1, 6].

QDs are inorganic crystal particles that have sizes in the range of 1-10 nm. In the present study, CdSe QD having size in the range of 2-4 nm was found to show quantum confinement effect due to the reduction in the semiconductor particle size less than the Bohr radius. This is evident from increasing energy band gap and conductivity of the composite material. QDs are used in electronic industry for different prospective applications as optical amplifier media for telecommunication network, and photovoltaic devices [2].

EXPERIMENTAL TECHNIQUES

Cadmium acetate dihydrate (98%), selenium (Metal) powder (99%), thiourea (99%), sodium sulphite (96%),triethanolamine (97%), liquid ammonia (25%) were procured from Thermo Fisher Scientific India Pvt. Ltd. & Central Drug House, New Delhi. Di-ionized water was used as solvent.

In the present study chemical co precipitation method was used to synthesis CdSe(S) Quantum dots using selenium metal, cadmium acetate, thiourea, and triethanolamine. Di-ionized water was used as solvent. The presence of triethanolamine (TEA) led to the reduction of the particle sizes by capping the precipitate particles. These particles being very small in dimension are called CdSe Quantum dots. The pH of the solution was maintained around 12.The precipitate so obtained was thencentrifuged at 9000 rpm for 10 min andwashed several times with distilled water and finally with acetone.The material so obtained was dried at 200˚C to get powdered CdSe(S) nanoparticles. These quantum dots were characterized using XRD by Bruker D8-Discover system using Cu-K_α radiation (λ=1.5406 Å). FTIR spectra were recorded using Jasco 660 plus Japan. UV studies were carried out using a double beam Shimadzu (model 2450) UV-VIS spectrophotometer. TEM studies were also performed using Transmission Electron Microscope [JEOL-1230].

RESULTS AND DISCUSSION

FTIR spectra [Fig.1 (a)] of CdSe shows the presence of OH bond (3429 cm^{-1}), stretching vibration of C=C (1627 cm^{-1}), C-O (1185 cm^{-1}& 1110cm^{-1}) and –C-H bending vibrations (1400 $cm^{-1)}$.The absorption peak at 618 cm^{-1}corresponds to CdSe nanoparticles [3].

XRD spectra [Fig.1 (b)], of CdSe(S) indicates the presence of both the phases, viz. cubic and hexagonal.The prominent peak (111) correspond to cubic phase at 25.54˚(JCPDS card no 19-019, 65-2891,77-2307). The Debye-Scherer formula (eq. 1) **[**4, 5**]** was used to calculate the average particle size of CdSe(S). The particle size was found to be 4.5nm,

$$D = \frac{0.9\,\lambda}{\beta\ cos\theta} \quad (1)$$

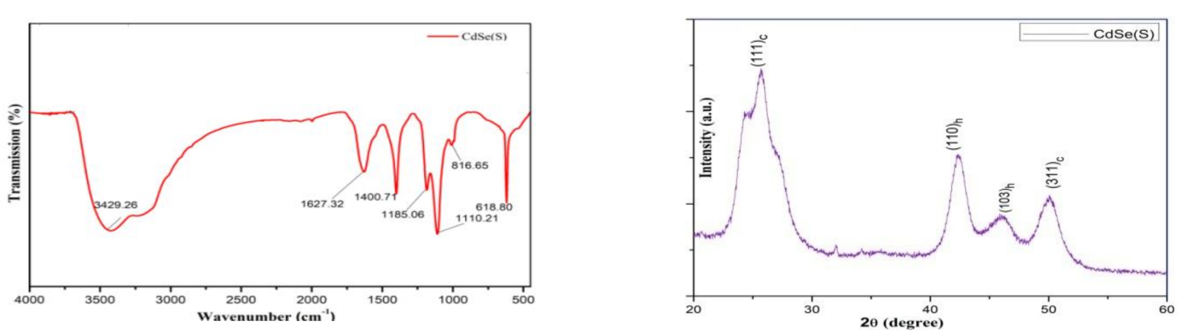
The crystallite sizes of CdSe(S) quantum dots corresponding to different peaks were found to be 3 nm, 5 nm and 6 nm, respectively. Theparticle size obtained by TEM was also in the range of 3nm to 8nm which agrees well with the XRD data. The results are summarized in Table 1. The calculated numerical values of lattice constant were found very close to the standard value (5.818 Å-JCPDS card no. 19-019). Broadening of XRD peaks shows polycrystalline nature of CdSe quantum dots.

Fig.2 (a) and 2(b) show the TEM picture of these particles having different morphology of CdSe(S) QDs. The shape of the particle is spherical having different diameters 4nm, 5nm, 7nm, 8nm respectively. The average diameter comes out to be 4.6nm, which best matches with XRD results. There is good consistency in between the TEM analysis and the XRD result as shown in table-1.

The absorption spectra of CdSe QDs are shown in Fig.3 (a). The absorption peak at shorter wavelength is due to size quantization effect in CdSe particles, which might be due to the reduction of particle size, the energy band gap (E_g) was calculated from the absorption spectra using the Tauc relationship (eq. 2)**[6]**, as given below:

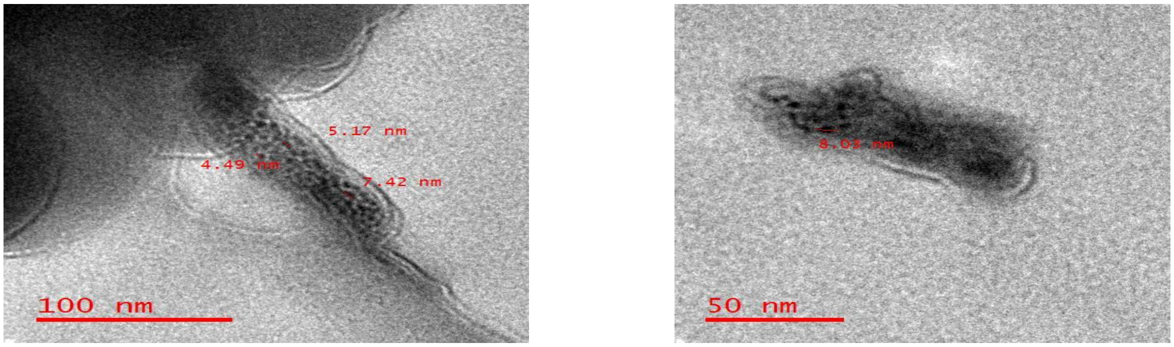
$$(\alpha h\nu) = A(h\nu - E_g)^n \quad (2)$$

Fig 3(b) shows the variation of $(\alpha h\upsilon)^2$ Vs hυ for CdSe(S) QDs. The optical band gap (E_g) was calculated by extrapolating the straight-line portion of $(\alpha h\upsilon)^2$ Vs hυ graph to hυ axis**.**The energy band gap calculated from these plots comes out to be 2.3eV. Lower energy band gap shows semiconducting nature of CdSe(S).



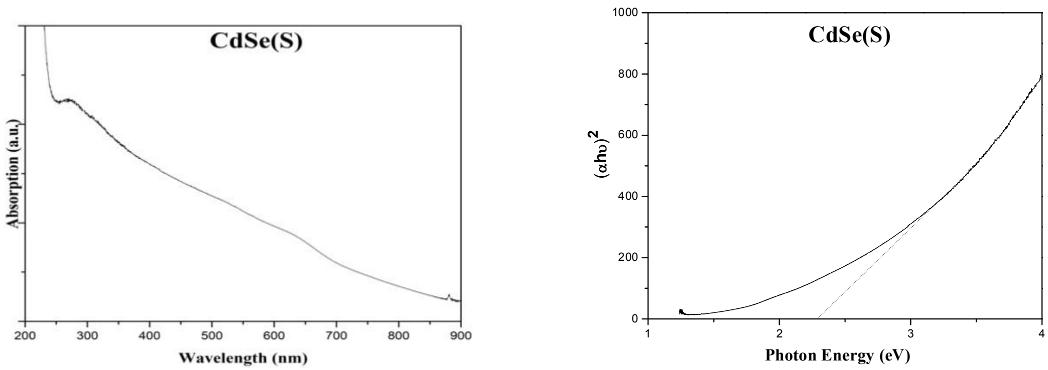
(a) (b)

FIGURE 1. (a) FTIR and (b) XRD spectra of CdSe QDs.



(a) (b)

FIGURE 2(a) and (b). TEM images of CdSe nanoparticles



(a) (b)

FIGURE 3. (a)Absorption spectra and (b) Energy band gap of CdSe(S) Quantum Dots.

TABLE 1. Structural parameter of CdSe(S) QD

Parameter	**CdSe**
Bragg's angle(2θ) (in degree)	25.5˚ ,42.4˚, 50˚
d (spacing) in (in Å)	d_1=3.5, d_2=2.1, d_3=1.8
FWHM (in degree)	2.783˚, 1.510˚, 1.826˚
Crystallite size(nm)	3 nm, 6 nm, 5 nm;
Average crystallite size (nm)	4.6 nm
Lattice parameter (a)(in Å)	6.03
Lattice strain	0.0536, 0.017, 0.017
[hkl]	[111], [110], [311]

CONCLUSIONS

The present study reports a facile and low-cost synthesis strategy of CdSe(S) Quantum dots via chemical co-precipitation method.XRD spectra suggestfor their polycrystalline nature and prominent peak corresponding to cubic structure of CdSe(S) quantum dots. The crystallite sizes of CdSe(S) quantum dots were found to be 3 nm, 5 nm and 6 nm, respectively.The particle size obtained by TEM analysis was in the range of 3nm to 8nm which agrees well with those reported by the XRD data.The results show that quantum confinement effect as the size of CdSe is smaller than the Bohr radius. Optical band gap of the CdSe QD was found to be 2.3eV.The results indicate that the material issuitable for optoelectronic devices, optical amplifiers for telecommunication network, solar energy conversion, Light Emitting Diode etc. Lower energy band gap shows semiconducting nature of CdSe(S).

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