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Synthesis and characterization of cadmium sulfide (CdS) quantum dots (QDs) for quantum dot sensitized solar cell applications

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Abstract : Cadmium sulfide (CdS) quantum dots were prepared at various time durations and deposited by chemical bath deposition (CBD) method. The structural, morphological and optical properties were studied using powder X-ray diffraction (PXRD), scanning electron microscope (SEM) and UV-Vis NIR analysis respectively. From the observed PXRD pattern the particle size was calculated using Debye Scherrer's method. The calculated particle size was 3.6 nm and the corresponding (hkl) plane was indexed as (002). The lattice parameter of the CdS QDs was calculated. The cell parameters are a = 4.14Å and c = 6.715Å which are well agreed with standard JCPDS data. Using CdS QDs quantum dot sensitized solar cells (QDSSC) were fabricated on FTO substrates. Sol-gel method synthesized TiO₂ nanoparticles, N3-Ruthenium dye, CdS quantum dots, I_3/Γ electrolytes and Pt as counter electrode were used for cell fabrications.

Keywords: Semiconductors, Quantum Dots, Semiconductor devices, Solar energy.

1. Introduction

Nanotechnology refers to the research and technology development at atomic, molecular and macromolecular scales, which leads to the controlled manipulation and study of structures and devices with length scales in the range from 1 to 100 nm. CdS is one of the most important II-VI semiconductor compounds, possessing excellent optical properties. A tremendous amount of effort has been devoted to the synthesis and optical property study of CdS related nanoparticles and quantum dots[1]. Quantum dots sensitized solar cell (QDSSC) is a promising alternative to conventional Si-based solar cells due to low cost and easy manufacturing. In recent years, quantum-dot (QD) chalcogenide semiconductors such as CdS, CdSe and CdTe have also been employed as sensitizers due to two specific advantages. First and foremost, the size quantization effect allows one to tune the band gap energy and visible response by simply varying the QD size. Another advantage is that these QDs open new ways to utilize hot electrons or generate multiple electron-hole pairs with one single proton through the impact ionization effect[2].

In recent years, many quantum dot (QD) materials were investigated and applied as the sensitizer replacing organic dyes in the dye-sensitized solar cell (DSSC). Some of the advantages of QDs are tunable energy gaps, ability of multiple exciton generation, photostability, low cost and high absorption coefficient, which is known to reduce the dark current and increase the overall efficiency of solar cells. QD materials can tune their band gap energy level and this characteristics offers new opportunity to improve the light harvest ability.

In the present investigation CdS QDs were prepared by chemical bath deposition (CBD) technique. The prepared QDs were characterized using PXRD, SEM and UV- Vis NIR analysis to identify the structure, morphology and band gap energy respectively. The QDSSC was fabricated using laboratorial prepared CdS QDs and commercially available TiO_2 nanoparticle, electrolyte and Pt.

2. Experimental procedures

For a typical synthesis, CdS quantum dots have been deposited in a glass substrate by using chemical bath deposition (CBD) method. The cationic precursor 0.1 M of Cadmium nitrate (Cd(NO₃)₂.4H₂O) was dissolved in 20 ml of ethanol (C₂H₆O) solution. Then, the anionic precursor 0.1 M of thiourea (CH₄N₂S) was dissolved in the same solution. The glass substrate was immersed in the prepared solution for 1 minute. Finally, the CdS film was dried in hot air oven for few minutes.

3. Results and discussions

3.1 Powder X-ray diffraction (PXRD) analysis



Fig. 1. PXRD pattern of CdS quantum dots by CBD method

Fig. 1 shows the PXRD pattern of the CdS QDs deposited by the chemical bath deposition (CBD) method. All the diffraction peaks in the pattern corresponds to the hexagonal phase of CdS. The lattice parameters have been calculated and it was found to be a = 4.14 Å and c = 6.715 Å. The obtained lattice parameter values are matched with previously reported literature and this is good agreement with the standard JCPDS data no. 89-2944. The presence of high intensity peaks ($2\theta = 26.108^\circ$) clearly shows that the particle size of CdS is very small and it was found to be 3.6 nm corresponding to the (002) plane. The particle size was calculated by using Scherrer's formula

$D = K\lambda/\beta cos\theta$

where K is the shape factor (0.9), β is the full width at half maximum (FWHM), λ - is the wavelength of CuK α_1 radiation (1.5406Å), θ is the Bragg's diffraction angle.

3.2 Scanning electron microscopy (SEM)

The surface morphology of the CdS QDs were analyzed using scanning electron microscopy (SEM) and the images of the QDs are shown in Fig. 2a and b. Spherical like structures were observed in CdS QDs prepared in chemical bath deposition (CBD) method. The crystalline natures of the observed particles are very good. From the figures. 2 (a) and (b) shows it is clearly the agglomerated phases were observed.

3.3 Thickness measurement

The thickness of Cadmium sulfide (CdS) Quantum Dots (QD) was carried out using thickness profilometer. The observed film thickness of CdS QDs was 0.12µm.



Fig. 2 (a) and (b) SEM images of CdS films deposited by CBD method



3.3 Optical absorption analysis

Fig. 3Absorption spectrum of CdS QDs deposited by CBD method



Figure. 3 shows that the optical absorption spectrum of CdS quantum dots deposited using chemical bath deposition method. In semiconductors, the relation connecting the absorption coefficient α , the incident photon energy hv and optical band gap E_g takes the form

where k is a constant related to the effective masses associated with the bands and m = 1/2 for a direct-gap material, 2 for an indirect-gap material and 3/2 for a forbidden-direct energy gap. From the optical absorption spectrum, it is clearly seen that the absorption edge of CdS quantum dots is being located at around 290-300 nm. Figure. 4 shows that the optical band gap energy figure of the CdS QDs. The obtained optical band gap energy (E_g) of CdS QDS is calculated using the equation (1). The estimated E_g value was in the range of 2.31 eV and the value is in very good agreement with the earlier literature reports[3].

4 Conclusions

In conclusions, CdS quantum dots were successfully prepared by a chemical bath deposition (CBD) method. According to the results of PXRD the particle size was calculated using Debye-Scherrer's method. The particle size was found to be 3.6 nm. SEM images confirm the spherical like morphology was observed and the morphologies are agglomerated. The film thickness was measured using thickness profilometer and the obtained thickness was 0.12μ m. The optical band gap energy (Eg) of CdS QDs was 2.31 eV.

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