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STRUCTURAL AND ELECTRICAL PROPERTIES OF SPRAY-DEPOSITED CdSe/TiO_2 NANOCRYSTALLINE THIN FILM

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Abstract:

Nanocrystalline thin films of CdSe/TiO_2 at optimal substrate temperatures were deposited on a fluorine-doped tin oxide glass substrate by spray pyrolysis. The structural and electrical properties were examined using X-Ray diffractometer, scanning electron microscopy, and Photoelectrochemical cell. The X- ray pattern revels the deposited and doped CdSe/TiO_2 thin films have polycrystalline in nature and hexagonal in structure. The SEM image shows agglomerated particles that appear flake-like or granular, characteristic of thin films grown at elevated temperatures. The Photoelectrochemical performance shows that the short-circuit current Isc is maximum 0.625 mA for CdSe/TiO_2 thin film and open circuit voltage is minimum (275 mV) under the illumination of light of tungsten 500W, this property can be used for photocatalysis by thin film.

Keywords: *Cadmium selenide, TiO_2, Thin Films, Spray Pyrolysis, Photoelectrochemical Cell.*

Introduction

One of most notable II-VI group semiconductors is cadmium selenide (CdSe), which has exceptional optoelectronic qualities. High resistance to photo-corrosion is exhibited by wurtzite (hexagonal structure) and zinc blende (cubic structure) crystal forms (1). Given its flexible energy gaps, nanocrystalline CdSe exhibits extraordinary electrical and optical capabilities (2). CdSe's potential for thin-film applications among II-VI semiconductors is highlighted by its strong photosensitivity and optical band gap of 1.74 eV at room temperature (1, 2). Patil *et al.* (3) produced CdSe thin films of varying thickness onto an amorphous glass substrate during the course of their attempts to manufacture CdSe thin films for a variety of applications. It obtains hexagonal structure with (002) plane and preferred orientation. 2.3 eV was determined to be direct band gap. Olusola *et al.* (4) deposited CdSe thin film on FTO-coated glass utilizing potentiostatic electrodeposition method film shown and n- type conductivity and optical band gap was estimated to be 2.00 and 1.80 eV. Talele *et al.* (5) deposited polycrystalline CdSe thin film on amorphous glass substrate by thermal evaporation method. With a hexagonal structure and a polycrystalline nature, the produced thin films have an optical band gap of 3.3 - 3.7eV. Mohammed *et al.* (6) deposited CdSe nanoparticles (NPs) by spin coating method the direct and gap obtained its 2.2 eV. Band gap increased because of quantum confinement effect. Hussain *et al.* (7) deposited low-temperature nanostructured CdSe thin film via chemical bath deposition method. Deposited thin film absorbs visible light into range of 563 to 585nm corresponds to band gap energy 2.12 and 2.20 eV. The reported techniques yield that can produce visible light energy for photovoltaic applications (8, 9).

The CdSe-sensitized TiO_2 nanoparticles has shown to improve the photo response in solar cell and efficiency in photocatalytic processes. Ho *et al.* (10) deposited CdSe and CdSe/TiO_2 thin fill by ultrasound driven method. CdSe in NPs acts as photosensitizer not only extend spectral response of TiO_2 to visible region, but also reduce charge combination. The blue shift confirms quantum confinement effect which makes electron ejection from CdSe to more efficient and increases degree of charge separation there by improving performance of photo catalyst. (11, 12)

TiO_2 is a promising semiconductor for water decontamination, but its low photonic efficiency is due to rapid electron-hole recombination. Research focuses on enhancing charge separation through photoelectrocatalysis, which combines electrochemical and photocatalytic processes (13, 14, 15). Applying an anodic bias to a TiO_2-based photoanode directs photogenerated electrons to a counter electrode via an external circuit, improving charge separation efficiency. Cadmium selenide (CdSe), with a lower band gap (1.7 eV) (16, 17) is a potential photocatalyst; however, its low surface area, fast recombination, and high-cost limit industrial applications. Combining CdSe with wide-bandgap semiconductors like TiO_2 enhances its photosensitizing properties, making it effective for organic pollutant degradation and environmental remediation (18, 19).

2. Experimental procedure

2.1 Materials and methods

The precursors for cadmium, selenium, and Titanium dioxide, Cadmium acetate [$Cd(CH_3COO)_2$], Selenourea [N_2H_4CSe], and Titanyl Acetylacetonate [$C_{10}H_{14}O_5Ti$] were utilized. Stannic chloride with chromium tetrachloride, ammonium fluoride, methanol, ethanol, and glass substrate etc. Sigma Aldrich is the source of all A.R. grade chemicals.

To eliminate any impurities that might interfere with film deposition process, substrates were thoroughly cleaned. To get rid of sticky oil, lint, and grease particles, they were first cleaned with Laboline solution. Following a water rinse, they were boiled in chromic acid for five minutes. After dissolving chromium tetrachloride (1g) in double-distilled water (100 cc), producing a chromic acid solution, chromium tetrachloride (3.5 g) was dissolved in double-distilled water (350 cc). Subsequently, the substrates underwent ultrasonic cleaning and further cleaning in double-distilled water (20).

2.2 Preparation of stock solution and fluorine doped tin oxide (FTO) thin film

Stannic chloride and ammonium fluoride were dissolved in 8 ml of propanol, with an additional 2 ml of methanol added for the preparation of the FTO thin film. The freshly prepared stock solution of 10 ml was mixed with 2 ml of methanol and 8 ml of propanol, resulting in a total solution volume of 20 ml. This solution was then sprayed onto conducting glass substrates to create the FTO thin film (20).

2.3 Preparation of CdSe thin film

The preparation of CdSe thin film involved the creation of precursor solutions for both Cd and Se. The Cd precursor was obtained by dissolving 0.0799 g of cadmium acetate in 20 ml of double distilled water to achieve a concentration of 0.015 M. Similarly, the Se precursor was prepared by dissolving 0.0369 g of selenourea in 20 ml of double distilled water, also resulting in a concentration of 0.015 M. The combined precursor solution totalling 40 ml was then sprayed onto fluorine-doped tin oxide substrates of size 0.125 cm ×2.5 cm ×7.5 cm through a specially designed glass nozzle. The resulting 40 cc precursor solution was sprayed through a specially designed glass nozzle onto the preheated glass substrates held at an optimized substrate temperature of 400°C. The compressed air was used as the carrier gas at a constant spray rate of 4 cc min^{-1}. The deposition parameters like solution concentration, substrate temperature, solution quantity, spray rate, nozzle to substrate distance (NSD), carrier gas flow rate, etc. was kept constant at optimized values. Then CdSe, in uniform, pinhole press and well adhesive films were formed and studied all properties. The deposition process was conducted at optimized temperatures 400 °C (20).

2.4 Preparation of CdSe/TiO2 thin films:

CdSe/TiO_2 thin film was prepared by dissolving 1.048 gm of Titanium Acetylacetonate as aprecursor of TiO_2 and is completely dissolved in 40 ml of methanol. Heterojunction thin films of CdSe/TiO_2 subsequently produced by spraying this solution over previously deposited CdSe thin films using following parameters: conc. 0.015 M, quantity 40 ml, and temperature at 470 °C at 10 kg/cm air pressure. (20)

2.5 Materials characterization:

The structural characterization of CdSe and CdSe/TiO_2 can be done by analysing the X-ray diffraction patterns obtained under Cu-Kα radiation from a Bruker D2 Phaser X-ray diffractometer made by Bruker analytical instrument Pvt. Ltd. The surface morphology was observed by scanning the electron microscope (JOEL-JSM 5600 operating at an accelerating voltage of 20 kV). The sheet resistance was determined by four probe measurements (Keithley Mode l2400). Photoelectrochemical characterization can be studied by PEC reactor cell.

3. Results and discussion

3.1 X-ray diffraction (XRD)

Non-destructive technique applied for various purposes such as phase identification, orientation determination, lattice parameter measurement, crystal quality assessment, and evaluation of crystal structure XRD is a widely used. In this study, the CdSe/TiO_2 thin films were characterized using an X-ray diffractometer (Model: D8 Advanced, Equipment code: 2734620) in the 2θ range from 0° to 90°, in order to examine the structural properties of the prepared thin films. The XRD of CdSe and CdSe/TiO_2 thin films deposited on FTO substrate are shown in Fig. 1ab.

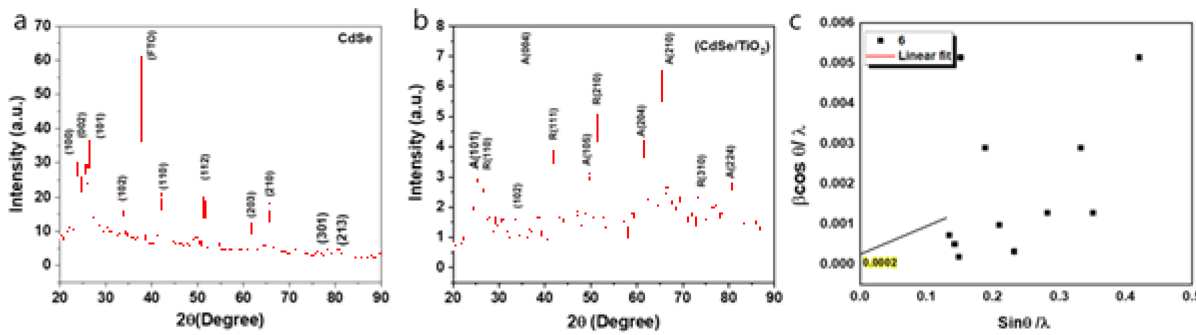

Figure 1: (a and b) XRD Pattern of CdSe and CdSe/TiO_2, and (c) W-H plot for CdSe/TiO_2 thin film

The spectra for pure CdSe JCPDF card no. 19-191, JCPDF card no. 03-065-5714 and JCPDF card no. 008-0459 were used for identification purposes. The broad hump that is observed in the background of XRD might be due to the characteristic peak (004) of TiO_2 in anatase phase. The XRD pattern of CdSe/TiO_2 shows many peaks, indicating the film has a polycrystalline character and has a hexagonal structure with the peak (004) being the most intense peak (20).

The average size of a crystal has been calculated from the Debye-Scherrer's equation,

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

Where λ is the wavelength of X-ray, β is called FWHM (Full Width at Half Maxima),θ is the angle of diffraction". The crystallite size was found to be 23.79 nm for CdSe and 39.87nm for CdSe/TiO_2 thin film. The increases in crystallite size might be due to higher deposition temperature at which allows the smaller crystallite to merge into larger one.

The interplanar distance spacing of lattice plane h, k, l was calculated by using Bragg's formula

$$d = \frac{\lambda}{2 \sin\theta} \qquad (2)$$

The average microstrain, which is defined as disarrangement of the lattice, was developed in the prepared nanoparticles calculated by using the relation as given below

$$\varepsilon = \frac{\beta \cos\theta}{4} \qquad (3)$$

The microstrain decreases for CdSe/TiO_2 thin film. The dislocation density was determined by using the equation,

$$\delta = \frac{1}{D^2} \qquad (4)$$

From the calculation it has been observed that the decrease in interplanar spacing, microstrain and dislocation density due to the strain is produced between the CdSe and TiO_2 at the heterojunction, which leads to a change in bond length and atomic arrangement. At higher deposition temperatures, CdSe nanoparticles experience a transition towards a more compact structure. Decreases in interplanar spacing lead to a change in the preferred crystallographic plane from (100) to (004). This is due to the deposition of TiO_2 onto CdSe, which introduces compressive strain on CdSe. Lattice mismatch leads to a preferred orientation change (21). All the parameters are discussed in Table 1.

Table 1: Lattice parameters for CdSe and CdSe/TiO_2 thin film

2θ (°)	**d (Å)**	**FWHM (rad)**	**Crystallite size (nm)**	**Plane**	**Microstrain ε**	**Dislocation density δ (nm)$^{-1}$**
23.79	3.74	0.0074	19.27	(100)	0.0018	0.002
37.86	2.37	0.0046	31.42	(004)	0.0011	0.001

The particle size was confirmed by using the Williamson-Hall equation as below,

$$\beta\cos\theta/\lambda = (K/D) + \varepsilon\sin\theta/\lambda \quad (5)$$

The plot of βcosθ/λ against sinθ/λ for CdSe and CdSe/TiO_2 thin film which is a straight line. The intercept on the y-axis gives the average strain and the reciprocal of intercept gives the average particle size determined using both methods are identical. The W-H plot is shown in Fig. 1c

3.2 FieldEEmission scanning electron microscopy (FE-SEM)

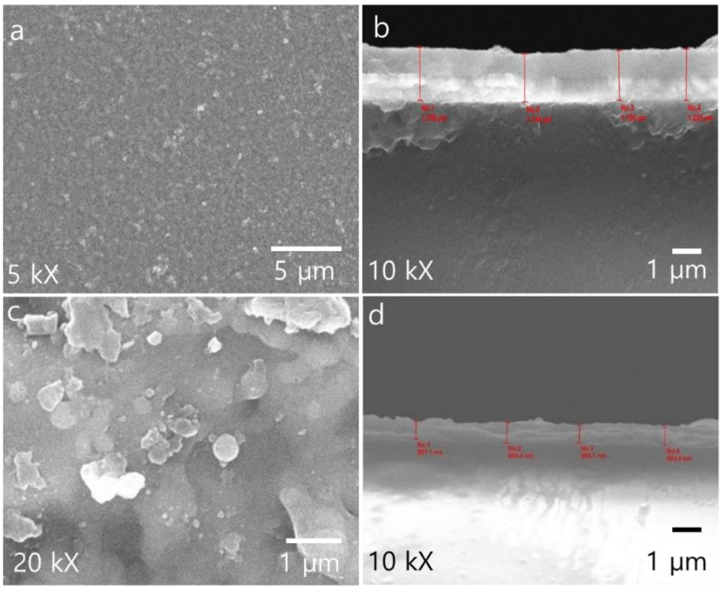

Figure 2: SEM images and cross section of (a and b) CdSe and (c and d) $CdSe/TiO_2$ thin films

In this study, SEM was utilized to investigate the morphological characteristics of $CdSe/TiO_2$ films. The SEM images revealed that the non-uniform distribution of particles with varying size (**Fig. 2a-d**). The background appearing relatively smooth suggesting the presence of thin film. The thickness of these thin films was calculated using cross section SEM as given in (**Table 2**). The SEM morphology suggests that the nanoparticles are embedded within a thin film matrix. The smaller particles seen may be CdSe nanoparticles, while larger bright regions could be agglomerated TiO_2 or CdSe clusters. Quantitative analysis of the SEM images determined the average particle size to be approximately 100.33 nm for CdSe and 98.27 nm for $CdSe/TiO_2$. This observation reveals that the particle size decreases due to the heterostructure, which introduces strain at the interface due to the difference in lattice parameters between CdSe and TiO_2. (20).

Table 2: The grain size and thickness for the CdSe and $CdSe/TiO_2$ thin film

Sr. No	Grain size of CdSe (nm)	Thickness of CdSe (μm)	Grain size of $CdSe/TiO_2$ (nm)	Thickness of $CdSe/TiO_2$ (nm)
1	117.7	1.082	99.3	591.0
2	105.5	1.120	92.71	654.4
3	89.73	1.119	81.8	586.1
4	88.39	1.094	119.3	603.1

3.3 Photoelectrochemical (PEC) characterization

The process of optimizing the preparation settings for high-quality adherent CdSe and $CdSe/TiO_2$ thin film is carried out by PEC characterization. The photoelectrochemical analysis was determined by measuring short circuit current (Isc) andopen circuit voltage (Voc) by photoelectrochemical cell (21) prepared by a polysulfide electrolyte of 1M concentration by adding 3.90 gm of sodium sulphite (Na_2S) and sodium hydroxide 1.99 gm in double distilled water 50ml and is completely dissolved then 1.60 gm of sulfur powder is dissolved in this solution. Now a thin film of deposited CdSe with an average surface area 7.5 cm x 2.5 cm is used as photoelectrode and a graphite as a counter electrode with thesame dimensions. It will be 0.5 cm between these two electrodes. Both theelectrodes are immersed in the polysulfide solution to measure the performance of CdSe thin by measuring Isc and Voc. characteristics on F.T.O. substrate under illumination with light with a tungsten lamp of 500W. The Photoelectrochemical cell set up is as given in Fig.3.

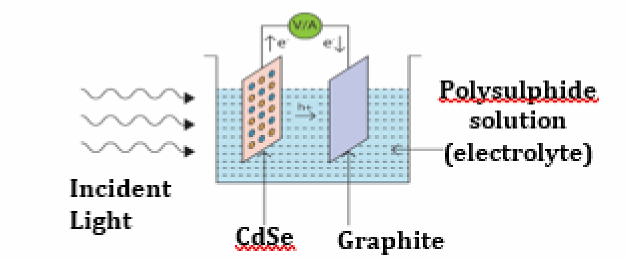

Figure 3: The Photoelectrochemical cell set up

Table 3: The short circuit current and open circuit voltage for CdSe and CdSe/TiO_2 thin film

Thin film	Isc (mA)	Voc (mV)
CdSe	2.2	340
CdSe/TiO_2	0.625	275

The decrease in short circuit current in CdSe/TiO_2 thin film is due to change is light absorption and recombination of charge carriers introduced by the heterojunction.

Conclusion

Nanocrystalline heterostructure CdSe and CdSe/TiO_2 thin films are deposited on FTO glass substrates using spray pyrolysis techniques. The XRD pattern of CdSe/TiO_2 shows many peaks, indicating the film has a polycrystalline character and has a hexagonal structure with the peak (004) being the most intense peak is the characteristic peak (004) of TiO_2 in anatase phase. SEM images show that particle size decreases due to the heterostructure, which introduces strain at the interface due to the difference in lattice parameters between CdSe and TiO_2. The Photoelectrochemical characterization confirms the decrease in photocurrent due to hetrojuction. This nanocomposite was employed for degradation of organic pollutant in waste water.

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