RESEARCH ARTICLE

CADMIUM SULPHIDE (CdS) DEPOSITION FOR CdTe-BASED SOLAR CELLS

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Abstract

Cadmium sulfide (CdS) is one of the most promising electron-transporting materials in CdTe-based solar cells. In the present study, we use chemical bath deposition (CBD) technique to synthesize cadmium sulphide (CdS). The influence of solution pH level on the structural properties of CdS films was studied using X-ray diffraction (XRD), Scanning Electron Microscopy (SEM) and Energy Dispersive X-ray Spectroscopy (EDS). X-ray diffraction (XRD) analysis revealed that the as-grown CdS thin films were polycrystalline in nature, consisting of hexagonal wurtzite phase. SEM images showed grains uniformly distributed over the surface of the substrates, and EDS results demonstrated that the composition analysis of Cd:S ratio is close to 1:1. These CdS layers are expected to enhance the current, resulting in best photovoltaic performance for CdTe-based solar cells.

Introduction:

Cadmium Sulphide (CdS) is a chalcogenide semiconductor II-VI compound of great interest due to its applications in solid-state physics such as n-type window layer for p-CdTe or chalcopyrite based solar cells p-CuInSe₂, and/or p-Cu(In,Ga)Se₂ (CIGS) (Komilov et al., 2018; Ramasamy et al., 2019). CdS thin films can be prepared in cubic, hexagonal and mixed phase structure (Ikhmayies et al., 2013; Xing-wei et al., 2011). It has been also reported that the cubic structure of CdS is a metastable one and transition from the cubic to stable hexagonal structure can be achieved by appropriate conditions. In addition, for solar cell applications, hexagonal phase is more preferred according to literature review (Abdolahzadeh Ziahari and Ghodsi, 2012; Maticiuc et al., 2014; Novruzov, 2013; Shaban, 2016). Up to date, there are several deposition techniques of cadmium sulphide (CdS) films that have been demonstrated experimentally their great interest. The following ones usually used are spray pyrolysis method (Faraj et al., 2019), chemical bath deposition (Waldiya et al., 2019), dip-coating technique (Pandya et al., 2017), electrodeposition (Alam et al., 2019), thermal evaporation (Isik et al., 2019), electron beam evaporation (Alamri, 2014), etc. Among these methods, chemical bath deposition (CBD) is the most efficient deposition technique reported in literature for cadmium sulfide films deposition due to its low cost equipment, very practical method which can be easily assembled locally in modest laboratory to yield films with good quality structure at low temperature (27-85 °C), etc.

The CBD is a technique in which thin films are deposited on substrates immersed in diluted alkaline solution containing metal ions and the chalcogenide source. This method usually uses a complexing agent to control the slow
release of metal ions (Cd\(^{2+}\)) and sulphur ions (S\(^{2-}\)) to produce the controlled homogeneous precipitation of the film on the substrates based on the chemical reactions. In the current research, we report the structural properties of CdS layers deposited on glass substrates by chemical bath deposition (CBD) technique from cadmium acetate precursor source. The essence of this work is to obtain good quality CdS layers that could be used as a window layer for the fabrication of high efficiency heterojunction cells of CdS/CdTe.

**Materials and Methods:-**

Materials used are cadmium chloride (CdCl\(_2\)), thiourea \([\text{CS(NH}_2\text{)}_2]\), ammonia (NH\(_3\)), ammonium chloride (NH\(_4\)Cl). Cadmium chloride of 0.125 M and thiourea of 0.35 M are employed as the cadmium ions and the sulfur ions sources respectively, and 10 M of ammonia is used as a complexing agent. First, we introduce 1.25 mL of cadmium chloride solution in 37.5 mL of de-ionized water. Then, 5 mL ammonia solution is added at the same time with 5 mL ammonium chloride solution in the range 0.01 - 2 M in order to adjust the pH level under the control of a pH-meter (pH = 10 - 12). In this research, three levels of pH were choosen (pH\(_1\) = 10.6, pH\(_2\) = 11.2 and pH\(_3\) = 11.8).

Cleaned glass substrates are inserted vertically into the bath and the solution was heated at appropriate temperature between 60°C and 85 °C. A magnetic stirring rod was placed inside the mixture to maintain the stirring rate at approximately 120 rpm. When, we achieve the desired temperature, 1.25 mL of thiourea solution is added under stirring condition to ensure homogeneous distribution of the chemicals. The total volume of solution is 50 mL. After deposition, the substrates are removed from the chemical bath, cleaned with de-ionized water and dried in conditional air. The formed films are yellow in colour.

The characterizations were mainly carried out using a scanning electron microscope (SEM Model 400 F) equipped with an energy dispersive X-ray spectroscopy (EDS). The crystalline phase of the films was studied using a XPERT-PRO X-ray diffractometer with a CuK\(\alpha\) anode (\(\lambda = 1.54060 \text{ Å}\)) operating at 35 kV and 30 mA. The diffraction patterns were collected at measurement temperature 25 °C and over an angular range of 10 to 60°. From the XRD data, the the average crystallite sizes (D) of the as-prepared films were estimated using the following equation (Cullity and Stock, 2001; Pandya and Raval, 2017):

\[
D = \frac{0.94\lambda}{\beta\cos\theta}
\]

Where \(\lambda\) is the wavelength of the X-ray radiation used, \(\theta\) is the Bragg diffraction angle of the XRD peak and \(\beta\) is the broadening of the diffraction line at half maxima measured in radian.

**Results and Discussion:-**

The XRD patterns of the as-syntheized CdS samples at different levels of pH (pH\(_1\) = 10.6, pH\(_2\) = 11.2 and pH\(_3\) = 11.8) are depicted in Figure 1. The diffraction peaks appear at 2θ values approximately equal to 24.8°, 26.6°, 28.2° and 43.6° corresponding respectively to (100), (002), (101) and (110) reflections. No other peak corresponding to cubic CdS is detected. All the reflection peaks correspond to the hexagonal wurtzite phase (space group P6\(_3\)mc) of CdS with lattice constants of \(a = 4.089 \text{ Å}\) and \(c = 6.548 \text{ Å}\), which matched with those in JCPDS card no: 41-1049 (Gevorgyan et al., 2016). As can be clearly seen, all the samples have highly oriented crystallites with a preferential orientation along the c-axis (002) perpendicular to the substrate plane. These observations are in good agreement with previous results (Gevorgyan et al., 2016; Hussein et al., 2019).
CdS films deposited from the solution with pH level 10.6 present the highest intensity peak (002), revealing the best crystallinity of films in this condition. Using equation (1), the average sizes of as-deposited CdS thin films derived from the data are estimated. The different values, as displayed in Table 1, are in good agreement with other results carried out in literature (Memarian et al., 2017; Priya et al., 2018).

**Table 1:** Structural parameters, average grain sizes and film thickness of CdS films

| pH level | $2\theta_{(002)}$ (°) | Average size, D (nm) |
|----------|----------------------|----------------------|
| 10.6     | 26.61                | 40.68                |
| 11.2     | 26.68                | 40.89                |
| 11.8     | 26.72                | 40.93                |

The surface morphology images for the CdS films are shown in Figure 2. SEM micrographs show that the films are uniform and have good adherence on the substrates. The differences in surface morphologies are apparent in the three cases. The film with pH3 shows the smallest grain size of the CdS layer. Similar morphology is earlier reported (Islam et al., 2013; Memarian et al., 2017). The sample, prepared at pH level 10.6 has the best surface morphology with the lowest aggregation which indicates that the formation of aggregation is due to the coalescence of the nanoparticles as pH level increases (Birkholz et al., 2006; Fadavieslam et al., 2017).

**Figure 1:** X-ray diffraction spectra of the as-deposited CdS thin films at pH level 10.6 (a), 11.2 (b) and 11.8 (c)

**Figure 2:** Plane-view SEM images of CdS thin films, deposited from solution pH equal to pH level 10.6 (a), 11.2 (b) and 11.8 (c)
The EDS data were analyzed for atomic composition and stoichiometry of the as-grown CdS thin films. The results are shown in Table 1. The composition analysis of CdS reveals that the Cd:S ratio is close to 1:1 which indicates that the CdS deposition periods were uniform in all the films.

| Solution pH level | Atomic (%) | Stoichiometry |
|-------------------|------------|---------------|
|                   | Cd         | S             |               |
| 10.6              | 53.29      | 46.71         | CdS\textsubscript{1.14} |
| 11.2              | 53.77      | 46.23         | CdS\textsubscript{1.16} |
| 11.8              | 53.92      | 46.08         | CdS\textsubscript{1.17} |

Conclusion:-
Cadmium sulfide (CdS) thin films were successfully deposited on glass substrates using chemical bath deposition (CBD) for three different levels of pH. XRD revealed hexagonal wurtzite crystalline structure. The average sizes of the grains are in the range of 40.68-40.93 nm. SEM images showed uniformity surface of the as-grown thin films and good adherence on substrates. EDS results confirmed that the composition analysis of Cd:S ratio is close to 1:1. These new CdS layers are expected to effectively enhance the current, resulting in best photovoltaic performance for CdTe-based solat cells.

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