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Technical Note

Optical Properties of Chemically Synthesized Cadmium Sulphide for Solar Cell Applications

M. A. SALAWU^a, A. B. ALABI^b, S. B. SHARAFA^c and T. AKOMOLAFE^b

^a Physics/Electronics Unit, P.M.B. 1371, Kwara State Polytechnic, Ilorin, Nigeria.

^bDepartment of Physics, University of Ilorin, Ilorin, Nigeria.

^c Department of Physics, Usmanu Danfodiyo University Sokoto, Nigeria.

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Abstract: This paper presents the optical properties of chemically synthesized cadmium sulphide for solar cell applications. CdS nano-particles were synthesized with chemical route method using cadmium sulphate as cadmium ion source and thiourea as sulphide ion source. The prepared CdS nano-particles were characterized with XRD and SEM. Then, the prepared CdS was deposited on well cleaned glass substrate by thermal evaporation technique to obtain a film of 100 nm thickness. The film was optically characterized with UV-Visible spectrophotometer and FTIR Spectrometer. The peaks at 43° and 52° indicate that the nano-particles contain a mixture of hexagonal (wurtzite) and cubic (zincblende) structures which confirmed the greenockite and the Hawleyite phases of CdS. The optical analyses showed high optical transmittance of 90 % at 658 nm, reflectance of 47.76 % at 488 nm and the absorbance of 0.165 A.U. at 400 nm wavelength. The optical energy band gap of 2.42 eV was also deduced for the film from Tauc's plot. The Fourier Transform Infrared Radiation (FTIR) showed different peaks that indicate the stretching and vibrations of O-H, CH₃, C-O and C-H of CdS against their respective wave numbers. The prepared CdS can be employed as a window layer for the fabrication of CdS/CdTe thin film solar cells.

Keywords: SEM, XRD, CdS, UV-visible spectrophotometer. PACS: 42, 81.

Introduction

Among various nano-particles, a great interest has been shown towards cadmium sulphide (CdS) nano-particles because of availability of discrete energy levels, sizedependent optical properties, tunable bandgap, a well-developed synthetic protocol and easy preparation technique with good chemical stability [1]. CdS nano-particles are categorized under the group chalcogenides and are a II-VI group of semiconductor nano-particles which shows size-dependent optical and electrical properties due to its high surface area to volume ratio and quantum confinement [2]. Due to its very high photosensitivity, CdS has usage in detection of visible radiations, in light emitting diodes, solar cells, photochemical catalysis, gas

sensors, various luminescence devices, optoelectronic devices and a range of biological application [3-6]. Cadmium sulphide (CdS) semiconductor is an excellent visible light detector among other semiconductors [7]. It is an *n*-type direct band gap semiconductor (Eg = 2.42 eV) which has been studied extensively because of its band gap, high absorption coefficient, reasonable conversion efficiency, good stability and low cost [8].

Cadmium sulphide (CdS) nano-particles have been synthesized by several researchers using chemical precipitation methods [9-14] and cubic hexagonal phase was identified with different grain sizes ranging from 7 to 16 nm [10-11] for the nano-particles and the films. Deposition of CdS nano-particles has been carried out by Chemical Bath Deposition technique [15-17] and Spray Pyrolysis technique [6], among others, to obtain thin film nanostructures with different morphologies, such as acicular-like, mesoporous, spherical shapes, and crystallite sizes varying from 11 to 16 nm had also been reported [11].

The synthesis and characterization of cadmium sulphide *via* different techniques have attracted considerable attention due to its potential applications. Nanometer-sized semiconductors exhibit structural, electronic, optical, luminescence and photo conducting properties very different from their bulk properties [13].

This paper investigates the optical properties of 100 nm CdS thin film from chemically synthesized CdS nano-particles deposited by thermal evaporation technique. This technique has the possibility of obtaining uniform and quality films with good adherence without inclusion of impurities. The percentage transmittance. reflectance and absorbance characteristics of this film shall be investigated for window layer in the fabrication of efficient CdS/CdTe thin film solar cells.

Materials and Methods

A. Synthesis of Cadmium Sulphide

- i. 0.05 M of cadmium sulphate (CdSO₄) was used as a Cd⁺⁺ ion source and 0.10 M of thiourea as the S⁻ ion source at a working solution of temperature $70 \pm 5^{\circ}$ C.
- ii. Ammonia solution was used to adjust the pH of the reaction mixture as a complexing agent. The variation of pH during the growth is important in the structural film quality.
- iii. The reaction mechanism involved in the formation process of CdS nano-particles can be formulated as follows:

$$3CdSO_4.8H_2O + H_2O \rightarrow 3Cd^{2+} + SO_4^{2-}$$
 (1)

 $Cd^{2+} + (NH_2)_2CS \rightarrow [Cd(NH_2 - CS - NH_2)]^{2+}$ (2)

$$NH_2 - CS - NH_2 + 2H_2O \rightarrow 2NH_3 + CO_2 + H_2S$$
(3)

 $[Cd(NH_2 - CS - NH_2)]^{2+} + H_2S \to CdS + (3)$ NH_2CSNH_2 + 2H⁺ (4)

$$nCdS \to (CdS)_n \tag{5}$$

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B. Deposition and Characterization of CdS Film

The prepared CdS nano-particles were characterized with X-Ray Diffractometer (XRD) and Scanning Electron Microscope (SEM). The prepared CdS nano-particles were evaporated from molybdenum boat and deposited on clean glass substrate as thin films form. The glass substrate was cleaned with detergent, acetone and methanol and washed in an ultrasonic bath with de-ionized water and then dried in a dustfree atmosphere. CdS thin film of 100 nm was ensured on the glass substrate with thermal evaporation technique, in a residual pressure of 10⁻⁵ torr. The substrate temperature was kept fixed at room temperature. Thermal evaporation uses an electric resistance heater to melt the material and raise its vapour pressure to a useful range. This is done in a high vacuum to allow the vapour to reach the substrate without reacting with or scattering against other gas-phase atoms in the chamber, as well as to reduce the incorporation of impurities from the residual gas in the vacuum chamber. The vacuum is required to allow the molecules to evaporate freely in the chamber and subsequently condense on the surface of the glass substrate. The film was characterized with UV-visible optically spectrophotometer and Fourier Transform Infrared (FTIR) spectrometer. The photometric measurements were carried out using UV-visible spectrophotometer to measure percentage reflectance and transmittance. Beer's Lambert law was also employed to obtain the absorbance of the CdS film. The FTIR spectrometer was employed to determine the functional group of the material under study.

Results and Discussion

The XRD pattern of the synthesized CdS nano-particles is shown in Fig. 1. The identification and assignment of the observed diffraction patterns were carried out using the JCPDS 41-1049 Hexagonal (H) and JCPDS 10-0454 Cubic (C) reference patterns (Pantoja, 2013). The peak (101) appears at approximately 29°, indicating that the phase is hexagonal or at least a mixture of hexagonal and cubic phases. The peaks at 43° and 52° indicate that the films contain a mixture of hexagonal (wurtzite) and cubic (zincblende) structures, which confirmed the greenockite and the Hawleyite phases, respectively.

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FIG. 1. XRD analysis of the synthesized CdS nano-particles.

The Scanning Electron Microscope (SEM) photograph of the synthesized CdS nanoparticles is shown in Fig. 2. The result display, some percentages of oxygen content in the particles which may be due to the presence of cracks or rather the cracks are a result of the oxidation occurring within the sample.



FIG. 2. SEM photographs of the synthesized CdS nano-particles.

Energy Dispersive (EDX) analysis of the chemically synthesized CdS nano-particles is shown in Table 1. The analytical errors of the

chemically synthesized CdS were reasonably low.

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TABLE 1. The elements' normalized weight percents of the prepared CdS nano-particles.

Element	Normalized [wt. %]
Oxygen	10.58
Silicon	0.9
Cadmium	74.66
Sulfur	13.65
Aluminum	0.16
Total	100

The percentage reflectance characteristics of the CdS film are visualized in Fig. 3 as a function of wavelength. It is found that the magnitude of reflectance of the CdS film varies periodically with wavelength. Multiple oscillations occur on the reflectance curves due to interferences among multiple reflected waves. As the wavelength increases, the oscillation period of the film also changes. Thus, the reflectance characteristics of the CdS film are strongly dependent on the wavelength of electromagnetic spectra. Highest peak value of 47.76 % occurred at 488 nm wavelength.

The percentage optical transmittance spectrum of 100 nm CdS film in the wavelength range from 400 to 800 nm is depicted in Fig. 4. The optical transmittance of CdS film increases from 69.35 % at 400 nm to 90 % at 658 nm wavelength. The result obtained is in agreement with the work of [18-19].

It is observed from the absorbance spectrum that the absorbance decreased with the increase in wavelength and found to be 0.165 at 400 nm wavelength (Fig. 5).

The optical band gap energies were evaluated by extrapolating the straight line of the Tauc plot for zero absorption coefficient ($\alpha = 0$). The optical energy band gap of 2.42 eV was obtained for the 100 nm CdS film (Fig. 6).



FIG. 3. % reflectance characteristics of 100 nm CdS film.



FIG. 4. % transmittance characteristics of 100 nm CdS film.



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FIG. 6. Band gap of 100 nm CdS film.

FTIR spectrum of 100 nm CdS film is shown in Fig. 7. In the higher energy region, the absorption band at 3724 per cm is assigned to O-H stretching of absorbed water on the surface of CdS. The absorption band at 1446 per cm is assigned to bending vibration of methanol used in the process. It is also verified by its CH₃stretching vibrations occurring as very weak just below 3000 per cm. The C-O stretching vibration of absorbed methanol gives its intense absorption band at 1373 per cm. Its ring C-H vibration occurs at about 3000 per cm, though, it is very weak. Similar such weak absorption band due to C-H bending vibrations was also observed at about 617 per cm. Hence, in addition to absorbed methanol on the surface of CdS, the presence of thiophenol in its dissociation form is also evident. These observations convincingly support the template role of thiophenol in the control of the size of CdS particles.



Conclusion

CdS nano-particles have been successfully prepared by chemical route method and identified by X-Ray Diffractometer (XRD). The peaks at 43° and 52° indicate that the nanoparticles contain a mixture of hexagonal (wurtzite) and cubic (zincblende) structures which confirmed the greenockite and the Hawleyite phases of CdS. 100 nm CdS film deposited *via* thermal evaporation technique showed a high optical transmittance of 90 % at 658 nm wavelength and a reflectance of 47.76 %

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at 488 nm wavelength. The absorbance of 0.165 A.U. was obtained at 400 nm wavelength and the optical energy band gap of 2.42 eV was deduced for the 100 nm CdS film from the Tauc plot. The Fourier Transform Infrared Radiation (FTIR) showed different peaks that indicate the stretching and vibrations of O-H, CH₃, C-O and C-H of CdS against their respective wave numbers. The prepared CdS can be employed as a window layer for the fabrication of CdS/CdTe thin film solar cells.

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