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INVESTIGATING THE STRUCTURE, MORPHOLOGY AND OPTICAL BAND GAP OF CADMIUM SULPHIDE THIN FILMS GROWN BY CHEMICAL BATH DEPOSITION TECHNIQUE

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ABSTRACT: Thin films of cadmium sulphide have been successfully deposited by chemical bath deposition (CBD) technique using a mixed aqueous solution of cadmium sulphate, thiourea, and triethylamine. The films were characterized using a variety of techniques. Powder X-ray diffraction analysis shows that the as-deposited thin film has the hexagonal (wurtzite) structure. Scanning electron microscope (SEM) micrographs show the film surface consists of clusters with a globular surface morphology. Energy dispersive X-ray diffraction (EDAX) analysis confirmed the film to be consistent with the formation of cadmium sulphide on silica glass slide. The band gap, determined from optical absorption spectroscopy, was 2.42 eV which is consistent with other published results.

Keywords: cadmium sulphide thin films, chemical bath deposition, structure, morphology, optical band gap

I. INTRODUCTION

Cadmium sulphide (CdS) is an important II – VI Semiconductor which has been extensively studied due to its wide variety of applications ranging from photovoltaic to luminescent devices. CdS normally exists in hexagonal (greenockite) or cubic (hawleyite) forms and at high pressure, CdS transforms to a NaCl (halite) type structure [1]. CdS has a direct band gap of 2.42 eV, which falls in the visible spectrum at room temperature [2].

Interest in CdS has been driven by its application in the manufacture of photovoltaic and other optoelectronic devices. It has been used as a partner for the fabrication of several types of thin film solar cells such as CdTe, Cu_2S, and $CuInSe_2$. CdS has suitable band gap, high absorption co-efficient and considerable energy conversion efficiency [3]. The reported efficiencies of $CuInGaSe_2$ and CdTe based solar cells (using CdS buffer layer) have reached 19.9 and 16.5 %, respectively [4, 5]. CdS is also used in the fabrication of other important devices such as photo sensors, laser materials, optical waveguides and nonlinear integrated optical devices [6, 7, 8]. CdS has also been known for many decades as a photocatalytic semiconductor material for solar hydrogen generation in the visible wavelength range [9].

There is considerable interest in the deposition of compound semiconductors by methods which involve relatively low capital expense and are technically undemanding on the experimentalist. A method which may meet the above criteria is Chemical Bath Deposition (CBD) [10, 11]. CBD takes advantage of the use of a reaction from a solution where different precursors can be dissolved easily either in the ionic or molecular form and react chemically on the substrates leading to film formation. The key advantages are low cost, large area and low temperature atmospheric processing [10]. Chemical bath deposition (CBD) is becoming an important deposition technique for thin films of compound materials like chalcogenides [12]. The film formation takes place from two distinct mechanisms: atom by atom growth or aggregation of colloids formed in solution by a homogeneous reaction. Cadmium sulphide grows according to the first mechanism and films are generally made of microcrystalline grains (size in the range 20 to 80 nm) presenting a hexagonal or cubic structure according to the composition of the solution and the nature of the substrate [13]. Although CBD has been shown to be particularly successful in preparing high quality CdS, with the mechanisms and kinetics extensively investigated [12] the concentrations of the components of the solution bath for CdS can be varied over a working range and each group use its own specific recipe, so there are as many recipes to deposit CdS as research groups working in the subject [14]. The surface morphology, structure and optical properties of CdS thin films depend on the deposition parameters, notably the concentration of the reactants, the pH of the solution, the bath temperature and the deposition time.

In this paper we report on the structure, morphology and optical band gap of CdS thin films grown on commercial silica glass substrate by chemical bath deposition technique, using a mixed aqueous solution of cadmium sulphate, thiourea, and triethylamine.

II. EXPERIMENTAL DETAILS

The starting materials used were cadmium sulphate (0.1 M), as a Cd^{2+} ion source, thiourea (0.5 M) as a S^{2-} ion source and Triethylamine (0.1 M) as a complexing agent. A mixture was prepared by dissolving the appropriate amount of $CdSO_4$, and TEA in deionised water. The pH of the solution was adjusted to 10 by drop-wise addition of ammonia. A Mettler Toledo InteLab@Expert Pro pH meter with temperature compensation and glass electrodes (calibrated against standard pH 4.01, 7.00 and 9.21 buffers) was used to record the pH of the solution, after which thiourea was added to obtain a final volume of 50 ml. Substrates were degreased and cleaned thoroughly using a standard procedure, before immersion in the chemical bath. The reaction mixture was stirred and maintained at a temperature of 70 ^oC for deposition. The coated substrates were removed after one and a half hours, washed with deionised water to remove loosely bound CdS precipitates and finally cleaned ultrasonically. As-deposited films were yellowish in colour and adherent. The substrates were allowed to dry under ambient conditions before film characterization.

The crystallographic structure of the film was analyzed with a Brucker D8 powder X-Ray Diffractometer (40 kV, 40 mA), using secondary graphite monochromated Cu-Kα radiation (λ = 0.15418 nm) source over the diffraction angle 2θ between 30^0 and 80^0. The scan time for each sample was three hours. The surface morphology was examined by a Philips XL30 FEG Scanning Electron Microscope (XL 30 series). The elemental composition of the sample was determined using an energy dispersive X-ray analysis (EDAX) attached to the scanning electron microscope. Films were carbon coated using a GATAN Model 682 precision etching coating system before carrying out the SEM and EDAX. Optical properties were measured at room temperature using a Cary 5000 (ver. 1.09) UV – VIS spectrophotometer within the wavelength range of 800 – 200 nm.

III. RESULTS AND DISCUSSION

A. X-Ray Diffraction patterns

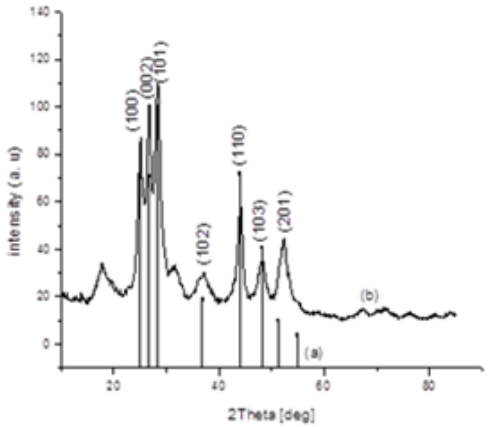

Figure 1: (a) JCPDS reference pattern 00-001-0789 for as-deposited CdS thin film

X-ray diffraction pattern of the as-deposited CdS thin film is shown in Fig. 1. A comparison of the peak positions (2θ values) with the JCPDS XRD spectra data for CdS [15] shows that the thin film has the hexagonal (wurtzite) structure with observed X-ray diffraction peaks corresponding to the (100), (002), (101), (102), (110), (103) and (201) planes. The hexagonal phase of CdS is formed under most film growth conditions [1]. In this study, powder X-ray diffraction produced no evidence for cubic CdS in the film.

B. Surface Morphology and Elemental Composition

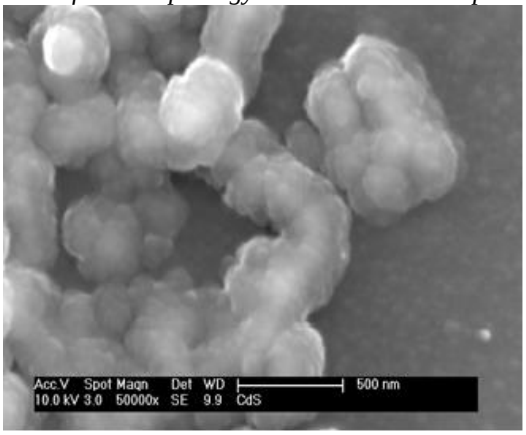

Figure 2a: SEM micrographs of the CdS thin film (magnification 50000x)

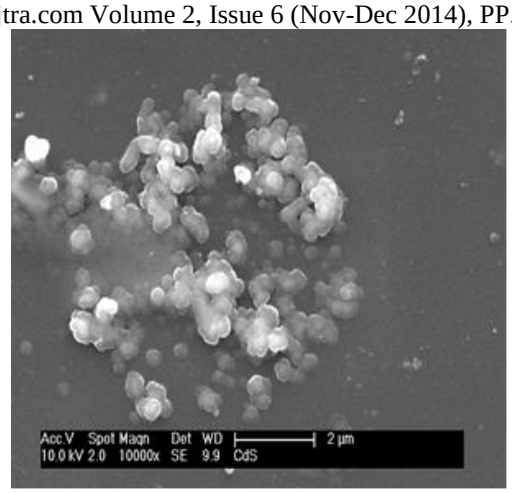

Figure 2b: SEM micrographs of the CdS thin film (magnification 20000x)

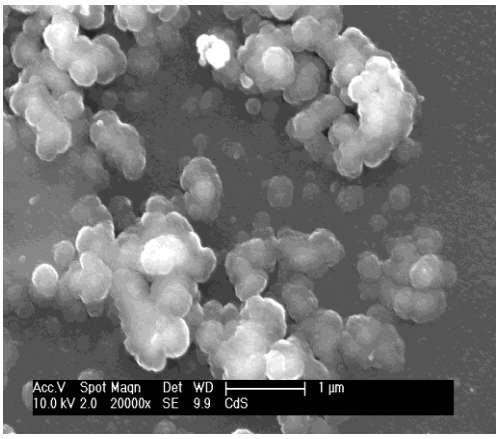

Figure 2c: SEM micrographs of the CdS thin film (magnification 10000x)

Figures 2a, 2b and 2c show the SEM micrographs of the as-deposited CdS thin film at different magnifications. The film surface consists of clusters with a globular surface morphology which agrees with the growth mechanism: homogeneous and heterogeneous reactions [16]. The composition of the CdS thin film deposited on glass substrate was analyzed by EDAX measurements with a power source of 20 kV. The EDAX spectrum of the film, shown in Fig. 3, confirmed the formation of CdS on silica glass slide. The presence of the large amount of impurities such as silicon, oxygen, magnesium, calcium and aluminium, emanate from the microscope glass slide used as the substrate.

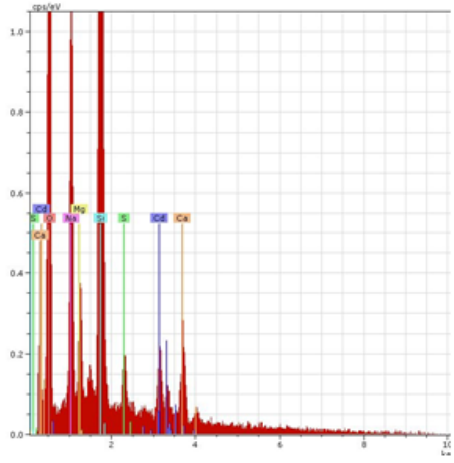

Figure 3: EDAX spectrum of as-deposited CdS thin film

C. Determination of the Optical Band gap

The optical band gap of the thin film was estimated from data obtained from optical absorbance versus wavelength with the Stern (1963) relationship of near-edge absorption which is given as [17]:

$$A = \frac{[k(h\upsilon - E_g)]^{n/2}}{h\upsilon} \quad (1)$$

where A is the absorbance, Eg is the band gap, v is the frequency, h is the Planck's constant, k is a constant while n carries the value of either 1 or 4. The value of n is 1and 4 for the direct transition and indirect transition, respectively. CdS is a direct band gap material, thus n is taken as 1. The band gap energy is obtained by extrapolating the linear portion of $(Ahv)^2$ versus hv to the energy axis at $(Ahv)^2 = 0$. Fig. 4 gives the band gap of the as-deposited CdS thin film.

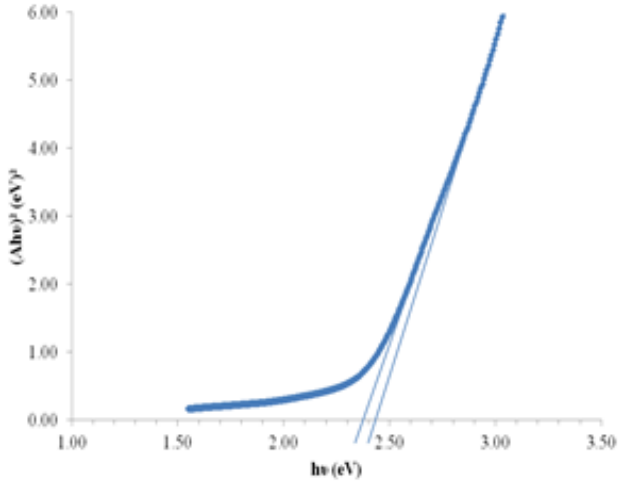

Figure 4: A graph of $(Ahv)^2$ plotted as a function of the photon energy, hυ, for CdS thin film.

Extrapolation of best fit line between $(Ahυ)^2$ and hυ to intercept the hυ axis at $(Ahυ)^2 = 0$ gives the band gap.

From Fig. 4, the extrapolations of the curves to the energy axis for zero absorption show the presence of two energy gaps: a lower one at 2.38 eV, which could be due to the presence of a defect state, and a higher one at 2.42 eV, which is the value quoted in literature as the band gap of CdS. A similar observation on the presence of two band gaps, one being a possible defect state associated with CdS, has been reported by Fan et al., [18] and several others.

IV. CONCLUSION

A well adherent thin film of cadmium sulphide has been successfully deposited on commercial glass slide substrate by chemical bath deposition technique, using a mixed aqueous solution of cadmium sulphate, thiourea, and triethylamine. The bath was kept at a pH of 10 and temperature 70°C for one and a half hours. Powder X-ray diffraction analysis shows that the as-deposited thin film has the hexagonal (wurtzite) structure. SEM micrographs show the film surface to consist of clusters with a globular surface morphology. EDAX analysis confirmed the film to be consistent with the formation of cadmium sulphide on silica glass slide. The band gap, determined from optical absorption spectroscopy, was 2.42 eV which is consistent with other published results. The effect of annealing on the morphology, structural and optical properties are under investigation and would be reported in subsequent publications.

V. ACKNOWLEDGEMENT

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