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Analysis of the Structural and Optical Properties of Thermally Evaporated Zinc Sulphide (ZnS) Thin Films for Photovoltaic Application

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ABSTRACT

Background: The conventional Cadmium Sulphide (CdS) buffer layer used on thin film solar cells contain toxic element Cadmium (Cd), which is not environmentally benign. The purpose of this analysis is to investigate the structural and optical properties of Zinc Sulphide (ZnS) thin films as an alternative and non-toxic buffer layer for thin film solar cell application. ZnS thin films were grown by thermal evaporation technique on soda lime glass substrates. Sample 1 and 2 were prepared by setting deposition current upto 25 A and 30 A, respectively. **Objective** The study of the structural and optical property of the prepared films was carried out by X-ray diffraction (XRD) and UV-Vis spectrometry. **Results:** Both the samples exhibit a peak at 2θ=28.50˚, corresponding to the (111) cubic structure as observed from XRD spectra. From the UV-Vis spectrometry, both the samples showed an average transmittance around 85% in the visible wave length. The bandgap has been found around 3.31 eV and 3.22 eV for sample 1 and 2, respectively. **Conclusion:** By analyzing the crystallographic properties and optical bandgap of the deposited thin films, it has been found that, ZnS can be considered as a potential alternative for replacing the conventional Cadmium Sulphide (CdS) buffer layer.

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INTRODUCTION

Generally Cadmium Sulphide (CdS) is used as a buffer layer for heterojunction thin film solar cells (Shao, Le-Xi, 2003). But from the environmental point of view, Cd has toxic effects on the environment. This fact has raised the necessity to look for environment friendly and non-toxic buffers layers (Wei, A., 2013). Several materials has been proposed as possible alternatives, such as: In_2S_3, ZnSe, (Zn,Mg)O and ZnS (Bouznit, Y., 2013). Zinc sulphide (ZnS) is considered as one of the most promising materials among these candidates (Hwang *et al*. 2012). It is a material which is environment friendly and does not contain any toxic element. Moreover it is cheap and abundant.

The use of an appropriate buffer/window material is crucial for obtaining a high efficiency solar cell (Ziabari, A.A., F.E. Ghodsi, 2013). Zinc sulfide (ZnS) is a direct wide bandgap, n-type II-VI compound semiconductor with the bandgap ranging from 3.5-3.7eV in room temperature (Nair, P.K., 1998). Low optical absorption in the visible and infrared spectral region and high refractive index are some unique properties possessed by ZnS, which makes it a widely used material in many optical and electronic areas (Wu, X., 2012). Compared to the bandgap (2.45 eV) of the conventional CdS buffer layer, ZnS has a higher bandgap which can enhance the blue response of the films and thus contribute to a better cell efficiency (Islam, M.A., 2012). In the literature, different techniques are found for preparing ZnS thin films. Such as: Chemical Bath Deposition (CBD), Spray Pyrolisis, Molecular Beam Epitaxy (MBE), RF Magnetron Sputtering, Thermal Evaporation, etc (Roy, P., 2006).

Thermal evaporation is a simple, fast, vacuum deposition process, which is very suitable for commercialization as well (Wang, K., 2010). In this work, we have used thermal evaporation technique for the deposition of ZnS thin films on top of cleaned soda lime glass substrates. The structural and optical properties of the deposited are studied elaborately in this analysis.

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Experimental Procedure:

Commercially available soda lime glass substrates were cleaned in ultra-sonic bath, degreased by methanol-acetone-methanol and de-ionized water for 15 minutes, respectively. The cleaned glasses were dried by dry N_2.

Then the glasses were attached in the substrate holder of the thermal evaporation chamber. A boat substrate distance of 4cm was maintained throughout the experiment. ZnS thin films were deposited on the cleaned glass substrates using high purity ZnS (Sigma Aldrich, purity 99.99%). Vacuum condition was attained inside the thermal evaporation chamber with the combination of rotary and diffusion pumps. After reaching a vacuum level of 10^{-6} torr, the amplitude of the dc current across the boat was gradually raised to heat ZnS powders to temperatures greater than the melting point. This allowed the evaporation of ZnS material. Sample 1 and 2 were prepared with maximum deposition current upto 25 A and 30 A, respectively. The deposition was carried out for 20 minutes in each case.

The structural and crystallographic properties of the grown films were investigated from the XRD data taken by 'BRUKER aXS-D8 Advance Cu-Kα' diffractometer. The optical properties like transmission, absorption and optical energy band gap of the films were studied by the 'Lambda 900 UV/Vis/NIR' spectrometer.

RESULT AND DISCUSSION

XRD Analysis:

The XRD patterns were obtained in the 2θ ranging from 20˚ to 60˚ using Cu-Kα radiation of wavelength, λ = 1.52 Å, for each samples.

Figure. 1 shows the XRD spectra found for sample 1 and 2, respectively. The XRD patterns confirm the polycrystalline nature of the films from the presence of the structural peaks in the XRD patterns.

In both cases a diffraction peak at 2θ = 28.50˚ is observed corresponding to the (111) reflection planes of the cubic phase ZnS. Although the only peak height of sample 1 corresponding to the (111) phase is smaller compared to the peak height found for sample 2 corresponding to the same phase. Another peak at 2θ = 47.9˚ is observed corresponding to the (220) phase. The prepared films are found to exhibit cubic or zinc blende structure. From the peak heights, it can be seen that, the intensity of the (111) orientation is predominant. But the small peak height of sample 1indicate a relatively low crystal quality compared to that of sample 2. The identification of the observed diffracted XRD patterns was done using the JCPDS data (JCPDS Card: 01-080-0020). In literature, ZnS thin films have been found to grow in cubic (zinc-blende) or hexagonal (wurtzite) structure In present work, we report the cubic (zinc-blende) structure of the ZnS material. The cubic ZnS structure is capable of reducing lattice mismatch between the buffer layer and quaternary compound semiconductor based absorbers..

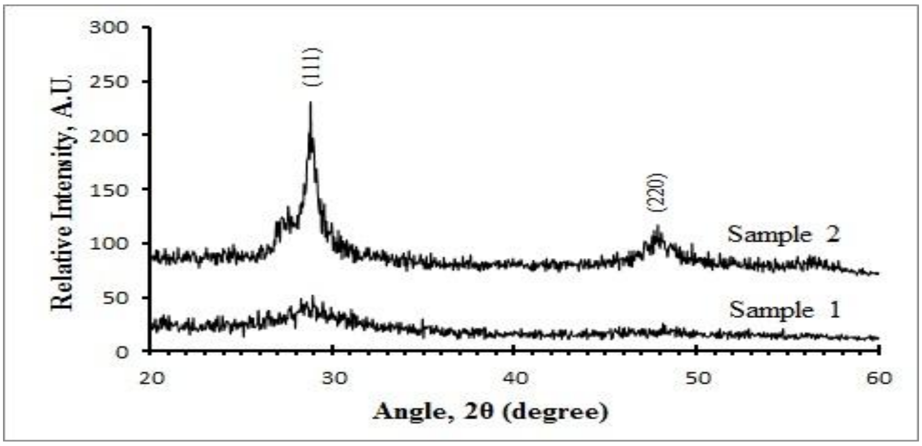

Fig. 1: XRD spectra of ZnS thin films.

Optical Properties:

The optical properties such as transmission, absorption and optical bandgap were investigated by UV-Vis spectrometry. During the transmission and absorption measurement, a commercially used blank soda lime glass slide was placed in one of the beam directions as the reference and another glass containing the deposited layer of ZnS was placed in the second beam direction. The data for transmission and absorption spectra ranging from 300 to 900 nm were obtained in this manner. The transmittance spectra for the grown films are shown in Figure. 2. The average transmittance for the thermally evaporated films are found to be 85% along the range, which confirms the suitability of the films to be used as a buffer layer in photovoltaic applications.

The bandgaps of the as-grown and annealed films were calculated from the following relationship (Tauc, J., 1974).

$$\alpha = A(h\gamma - E_g)^{1/2} / h\gamma \quad (1)$$

where, α is the absorption coefficient; A is a constant; $h\gamma$ is the energy of incidentphoton and E_g is the bandgap. The plot of $(\alpha h\gamma)^2$ versus hγ for the filmsare shown in Figure. 3. The bandgap energy is obtained by extrapolating the straight line portion of the graph to zero absorption coefficients. The intercept on the energy axis indicates the value of energy bandgap (Mariappan, R., 2012). From Figure. 3, the bandgap for sample 1 is found as 3.31eV. But for sample 2 the bandgap value reduced to 3.22eV.

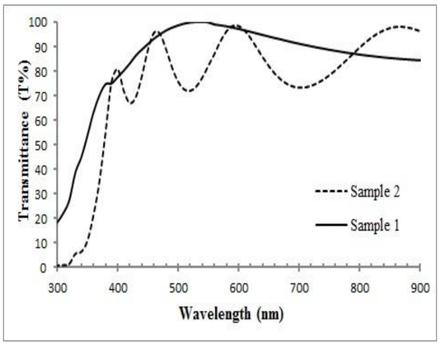

Fig. 2: Transmittance spectra.

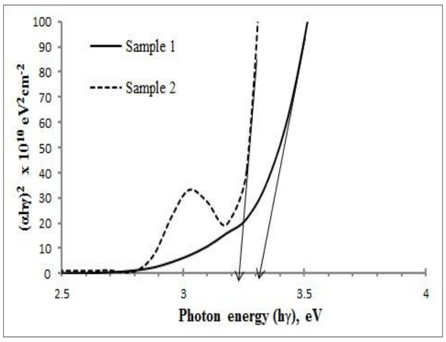

Fig. 3: Bandgap extrapolation.

Conclusion:

A study on the structural and optical properties of ZnS thin films grown at different deposition currents has been studied in this work. All the deposited films exhibited polycrystalline nature, showing a common peak at 2θ=28.50˚, which corresponds to the (111) cubic or zinc-blende phase. However, the increased peak height for the films grown at 30A deposition current indicates better crystallinity. The average transmittance of 85% proves the suitability of the films to be used as buffer/window layer for heterojunction thin film solar cells. The highest bandgap value of 3.31eV is found for the films grown by deposition current upto 25A. Although for the films, grown by deposition current upto 30A is better in terms of crystallinity, but it has shown lower bandgap compared to the previous one.

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