Solar Energy 167 (2018) 172–178

Contents lists available at ScienceDirect

Solar Energy

journal homepage: www.elsevier.com/locate/solener

Optical and electrical characterization of vacuum deposited n-CdS/n-ZnS bilayers

Rashmitha Keshav, M.G. Mahesha*

Department of Physics, Manipal Institute of Technology, Manipal Academy of Higher Education, 576104, India

ARTICLE INFO

Keywords:
II–VI semiconductors
Physical vapor deposition
Photoluminescence
I-V characteristics

ABSTRACT

A crucial comprehension of homopolar n-CdS/n-ZnS heterojunction is a key to design a solar device. Present study focuses on vacuum evaporated antireflective homopolar heterojunction with better spectral response as compared to single layer CdS. ZnS in combination with CdS facilitates minimized interface recombination losses and helps to attain large band bending by limiting conduction band spikes. With different thickness combinations of heterostructure, deviation in material properties such as lattice constant, band gap, has been observed. This further causes strain, defects, interface states, surface recombination centers and inter-diffusion leading to associated electro-optical changes. Thickness combination dependency of I-V properties of n-CdS/n-ZnS stack were numerically investigated using a new simulation software (wxAMPS) and examined with the experimental; where junction parameters were extracted using thermionic, Cheung's, and Norde models. Complexities faced in few thickness combinations which could hinder the ideal window character is also identified. The thickness combination with the lowest series resistance is presently referred to possess minimal resistive loss and high optical throughput.

1. Introduction

Generation of electricity from renewable sources is progressively recognized to play a significant purpose for the accomplishment of a variety of energy policy goals, such as improved security and diversity of energy supply, reduction of pollutants and greenhouse gas emission. This focuses the solution of the energy crisis on wise utilization of rich inexhaustible energy resources, such as solar, wind, geothermal, biomass and tidal energy. Each sort of alternative energy has its own advantages, disadvantages and applications (Sen et al., 2015). The common solar radiation received by the planet earth's surface, AM 1.5, is extremely abundant in photons with energies starting from 1.4 to 3 eV (Oladeji et al., 2000). CdTe, an important member from II to VI family, is best suited as absorber layer for this energy range. In conventional CdTe solar cells, CdS is prevalently used as a n- type heterojunction companion window. The band gap of CdS (2.4 eV) Oladeji et al., 2000 implies exclusive photons of energies in this range can reach to the absorber layer further contributing to the cell's photocurrent. Hence, several research groups have studied on cadmium based binary and ternary chalcogenides for photovoltaic applications(Nguyen et al., 2015; Ferekides et al., 2004; Abbas et al., 2018; Santhosh et al., 2017). As the absorption coefficients of chalcogenides are high about 10^4–10^5 cm^{-1} Oladeji et al., 2000, carrier generation by higher energy photons in n-type CdS window layer occurs at the surface i.e., far from depletion region where the yielded carriers can be collected. This normally results in the carrier loss to the surface recombination current leading to the reduction in photo-current and consequent increment of dark current. So, the challenge is to avoid short circuit effects and need of the hour is to allow high transmission, but hindrance is faced due to the thickness and band gap of CdS window layer.

To achieve the goal, one of the methods can be the direct reduction of CdS layer thickness. Decrease in the thickness (< 250 nm) which is routinely done to minimize the recombination current caused by the absorption, in another way leads to the non-uniformity and creation of pin holes after annealing treatment resulting in creating unwanted shunting paths which intern lowers the important solar cell parameters including efficiency. In addition, diffusion of CdS into CdTe during the process of fabrication of solar cells also must be accounted. As a solution, the idea of incorporation of buffer layer having the band-gap wider than CdS comes into picture where CdS layer thickness can still be maintained < 250 nm without compromising solar cell parameters. ZnS is the semiconductor which virtually fits the need. As ZnS band gap is 3.7 eV (Oladeji et al., 2000), it allows more photons from short wavelength regime to pass through it. Nevertheless, ZnS cannot be used as a mono layer window of CdTe solar cell. This is due to the fact that lattice mismatch between ZnS and CdTe is about 16% (Han et al.,

---

* Corresponding author.
E-mail address: maheshamg@gmail.com (M.G. Mahesha).

https://doi.org/10.1016/j.solener.2018.04.013
Received 19 February 2018; Received in revised form 2 April 2018; Accepted 5 April 2018

2013). Moreover, ZnS is highly resistive and hard to dope (Oladeji et al., 2000) which significantly increases the cell series resistance proving it to be a poor hetero-junction partner (Han et al., 2013). Hence the alternative solution to the above referred problem could be through optimizing the thicknesses of stacked n-CdS/n-ZnS bilayer to the CdTe solar cell without compromising in short wavelength spectral response, transport properties, shunt and series resistance of the cell. The behaviour of thermally grown n-CdS/n-ZnS junction are largely unexplored. In the present report, ZnS is stacked over CdS for various thickness combinations and optimization of the bi-layer thickness is done on a basis of essential characteristics of an ideal window layer which are assessed through transmittance spectra (T%), photo-luminescence (PL), structural analysis i.e., XRD and SEM followed by the electrical analysis.

2. Experimental details

Nano-crystalline n-CdS/n-ZnS thin films of different thickness combinations have been deposited on acid treated glass substrates by thermal evaporation via resistive heating method at base pressure of 2×10^{-6} mbar. Films have been grown by maintaining the substrates at room temperature and using stoichiometric powders of each compound (99.99%) separately as source materials in 200 A molybdenum boats. Investigated hetero-structures were fabricated without breaking the vacuum to avoid the oxide layer formation and grown at optimized rate of 0.2–0.3 nm/s as monitored by quartz crystal sensor set at 6 MHz (DTM-10). The synthesized n-CdS/n-ZnS bilayers of thickness combinations (in nm) 250/50, 200/100, 150/150, 100/200 and 50/250 were named as S_1, S_2, S_3, S_4 and S_5 respectively.

Optical transmittance was recorded at wavelength ranging from 400 to 1100 nm using double-beam Shimadzu UV-1800 PC spectrophotometer. The photoluminescence measurements were carried out using Agilent Cary Eclise WinFLR photoluminescence spectrometer. XRD using Rigaku Miniflex - 600 (Cu Kα at 40 kV, 15 mA), SEM model Zeiss EVO18 were employed to examine the crystal structure and cross section of the films. The I-V characterization of n-ZnS/n-CdS were carried out using Keithly 2450 source meter under dark conditions with aluminium as contact electrode on either side. Numerical modelling of bilayer was done by wxAMPS which is used to test the viability of proposed structure, predicting the effect of changes in material properties and allowing further analysis. Being an updated version of AMPS, wxAMPS conformed to similar numerical descriptions of defects and recombination, and added the effects of tunnelling current (Zhu et al., 1999; Liu et al., 2012).

3. Results and discussion

3.1. Optical characterization

Fig. 1a represents the optical transmittance spectra (Inset: PARAV fitted) recorded for various thickness combinations of n-CdS/n-ZnS. Software tool “PARAV” is used to obtain interference free transmission spectra (Ganjoo and Golovchak, 2008). All the thickness combinations have shown more than 70% transmittance beyond the absorption edge. Bilayer sample S_3 showed highest transmittance i.e., above 85% fitting the need of the window layer which can be attributed to the reduction in the structural defects, strain and improved crystallinity comparatively to the remaining thickness combinations. As the ZnS layer thickness increased the edge shifted towards lower wavelengths (blue shifted). Current window system is composed of two layers of different compound semiconductors corresponding to different band gaps, deposited on to a non-absorbing substrate such as glass. Here the upper layer (ZnS) has a wider band gap compared to the second layer (CdS). Near normal incidence, light rays suffering multiple reflections in the upper ZnS resulted in interference pattern recorded as maxima and minima confirming the uniformity of the grown films.

In Fig. 1b, it is clearly shown that n-CdS/n-ZnS bilayer has widened the transmission window as compared to the CdS monolayer with shift of absorption edge towards higher energy exhibiting an improved spectral response. Thus, for CdTe solar cells with bilayer window, a higher short-circuit current is anticipated as a result of higher transmittance at window region.

Fig. 2a shows the room temperature photo-luminescence (PL) spectra, recorded to examine the effect of thickness combinations of n-ZnS/n-CdS, with excitation wavelength 530 nm (2.34 eV). Usually, luminescence spectroscopy is very sensitive to small changes of the surface chemistry in chalcogenide nanoparticles where fate of photo-generated electron–hole pair is critically tied to semiconductor material applications. PL is a tool which provides the insight of intrinsic and radiative recombination associated with imperfections acting as traps in carrier transport. Minor defects in the semiconductor like vacancies, impurities or adsorbates at the surface produce the creation of trap states into which photo-excited electron can fall, or hole can float. Depending on the excitation energy, several transitions may occur, where the carriers are known to be in quasi-equilibrium state and their distributions can be represented by invoking quasi-fermi levels (Murugadoss, 2012). The resultant photoluminescence spectra thus, be quite Stokes-shifted from the absorbance spectra, depending on the energies of trap states compared to valence band and conduction band edges.

Manifested spectra covered a broad luminescence spectral range with the prominent emission band identified as L_{S1} at 645 nm (1.92 eV, red emission) and L_{S2} around 665 nm (1.86 eV, red emission) for combinations with lower ZnS thickness. According to the available literatures, emission observed at1.92 eV could be assigned to Zn interstitials (Zn_i). The broad peak L_{S2} can be a result of deep level defects due to the radiative transitions generated from crystallographic defects or surface states by S vacancy (V_S) or Cd interstitials (Cd_i) (Bakhsh et al., 2016; Varley et al., 2013). The increased thickness of ZnS layer is confirmed by the disappearance of the emission band L_{S2} as the absorption edge moved towards lower wavelength in accordance with transmittance spectra. Considerable reduction in the PL intensity of peaks for sample S_3 can be attributed to the comparative reduction in defects. The CIE plot for different thickness combinations are represented in Fig. 2b showing significant shift in the emission color. This indicates that thickness can be used as luminescence tuning tool. CIE plot demonstrated that increment in CdS thickness results in redshift whereas with ZnS thickness; blue shift. Sample S_3, being in lower wavelength, possibly has the better short spectral response and expected to have a positive effect on the performance of the solar cell.

3.2. Structural and morphological characterization

Structural information of the films is obtained through XRD. As shown in Table 1 sample S_3 combination is subjected to detailed structural analysis by comparing its structural parameters with that of 300 nm thick CdS and ZnS monolayers. Fig. 3a shows double diffraction peaks found at 2θ = 27.18° and 29.24° which are assigned to (1 1 1) plane and indicates highly preferential growth along this direction exhibiting cubic phase in agreement with the single layers. Position, height and width of the peak in diffractogram are the key parameters that can be used to extract the structural information of the films subjected to study. The average crystallite size is estimated by the width of diffraction peak at half maximum intensity (β) using Debye-Scherer formula (Fairbrother et al., 2014).

$$D = \frac{0.94\lambda}{\beta\cos\theta} \tag{1}$$

where θ is angle corresponding to the diffraction peak, λ is wavelength of radiation used.Strain developed in the films has been determined by Prathap et al. (2008);