Co-Sublimated Polycrystalline $Cd_{1-x}Zn_xTe$ Films for Multi-junction Solar Cells

Tushar Shimpi[1], Drew Swanson[2], Carey Reich[1,2], Jason Kephart[1], Anna Kindvall[1], Ramesh Pandey[3], Zachary Holman[2], Kurt Barth[1] and Walajabad Sampath[1]

[1]Department of Mechanical Engineering, Colorado State University, Fort Collins, CO 80523, USA
[2] School of Electrical, Computer and Energy Engineering, Arizona State University, Tempe, AZ, USA
[3] Department of Physics, Colorado State University, Fort Collins, CO 80523, USA

Abstract — **There are two major hurdles in the fabrication of top cell using polycrystalline films of CdTe alloys. First, the deposition of the films is difficult due to the difference in the vapor pressure of the individual elements present in the alloy or longer process time making it not economical. The retention of the original stoichiometry of the CdTe alloy after the $CdCl_2$ treatment is the second hurdle. In this work, polycrystalline films of $Cd_{(1-x)}Zn_xTe$ (Cd-Zn-Te) were fabricated with different band gaps by co-sublimation of CdTe and Zn. A strategy to retain the composition of the polycrystalline Cd-Zn-Te films is investigated and demonstrated. Quantum efficiency of greater than 0.7 was observed in the fabricated devices and band gap was maintained.**

***Index terms*- CdZnTe, top cell, tandem, high band gap CdTe alloy**

I. INTRODUCTION

A high band gap material is required in the top cell of a multi-junction solar cell to reduce thermalization and increase device voltage. The simulations carried out for optimal two stack multi-junction solar cell indicate that the top cell should have a band gap of 1.72 eV [1]. Materials such as perovskites [2] or from III-V group [3] can be tuned to the band gap of 1.72eV, but the devices fabricated from these materials are either unstable or problematic for large scale production.

The composition of ternary alloys of CdTe (Cd-Zn-Te, Cd-Mg-Te and Cd-Mn-Te) can be tuned to obtain a suitable band gap for the top cell in a multi-junction solar cell [4]–[7]. The fabrication of polycrystalline films using sublimation [8] of mentioned CdTe alloys are hindered because of the large differences in the vapor pressure of the individual elements during the deposition process. The deposition methods like sputtering [5], co-sputtering [9] and MOCVD [10] have been used. However there are concerns regarding uniform composition over large areas and lower throughput. The $CdCl_2$ treatment referred as passivation or activation treatment is an essential post deposition process carried out on CdTe devices to remove the defects in the film and improve the device performance [11], [12]. When applied to CdTe alloys, the change in the film composition during the $CdCl_2$ treatment to lower band gap material closer to CdTe due to loss as a volatile compound ($ZnCl_2$, $MgCl_2$, $MnCl_2$) is well documented [13][14][15][16].

In this work, polycrystalline films of Cd-Zn-Te with different band gaps were deposited by co-sublimation of CdTe and Zn. The composition of deposited films was varied by controlling the source temperature of zinc source. The sample with Cd-Zn-Te film with band gap of 1.72 eV was selected for device fabrication using a barrier of alumina during the $CdCl_2$ treatment to mitigate loss of Zn from the film. The alumina barrier was etched after the $CdCl_2$ treatment.

Optical and material characterization was conducted on as-deposited Cd-Zn-Te films with different band gaps. On the fabricated device, external quantum efficiency (EQE) measurements were carried out under different biasing conditions.

II. FABRICATION OF Cd-Zn-Te FILMS

The Cd-Zn-Te films were deposited in a superstrate configuration. The superstrates were Tec10 glass samples obtained from Pilkington glass and were soda-lime glass coated with Transparent Conducting Oxide (TCO) of SnO_2:F on one side. Before the deposition of Cd-Zn-Te, $Mg_{0.23}Zn_{0.77}O$ (Mg-Zn-O) layer was RF sputter deposited on TCO. The RF power applied to the target was 78.53 W/cm^2 and the size of the target was 10 cm. The composition of Mg-Zn-O was optimized for the band alignment with CdTe [17].

The schematic of co-sublimation source is shown in the Fig. 1, was developed by Colorado State University for fabrication thin films of different alloys such as Cd-Mg-Te [7] and Cd-Se-Te [18].

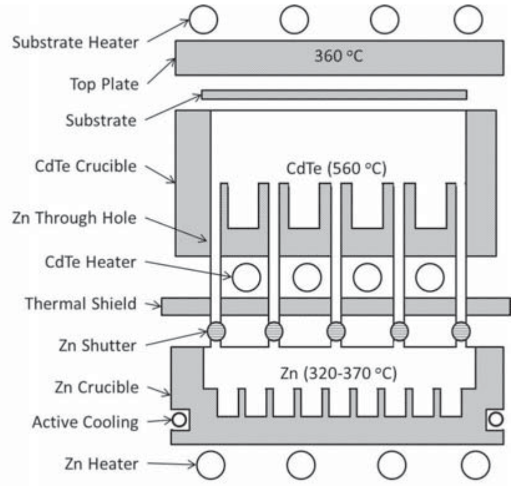


Fig. 1. Schematic of co-sublimation source for fabricating Cd-Zn-Te films.

Prior to deposition, the Tec 10 glass samples with Mg-Zn-O were heated individually and then transferred to the co-sublimation source without breaking vacuum. The process pressure of 40 mTorr was maintained in the vacuum chamber and ultra-high purity Ar gas was used to minimize oxidation.

The CdTe source temperature was maintained at 560^{o}C. The temperature of the zinc source was varied from 320^{o}C to 370^{o}C in small increments. On each superstrate, Cd-Zn-Te film of 1 um thick was deposited at various zinc source temperatures with the shutter in completely open position.

Alumina (~30 nm) was RF sputtered on the back of the Cd-Zn-Te (1.72 eV) film. The CdCl$_2$ treatment, copper doping, back contact and device delineation was conducted and is described elsewhere [19]. After the CdCl$_2$ treatment, alumina was etched using trimethyl-ammonia hydroxide, prior to contact deposition and device delineation.

The characterization of the deposited films was carried out by optical transmission and Glancing Angle X-ray Diffraction (GAXRD). In the optical transmission measurements, the wavelength was scanned from 350 nm to 1000 nm on a UV/VIS/NIR spectrophotometer by OceanOptics Inc. The transmission intensity recorded for different Cd-Zn-Te samples was used to calculate the band gap of the deposited film by Tauc plot method. For GAXRD measurements on Bruker D8 system, the glancing angle was 1^{o} to the incident X-ray beam generated by a copper source (λ = 1.5406 Å). The detector was swept from 20^{o} to 80^{o} to collect the diffracted X-rays from the deposited films. For EQE signal, the wavelength was scanned using a monochromator from 350 nm to 1000 nm in 10 nm increments and the device was biased under -300 mV, 0 mV, +200 mV and +300 mV.

III. CHARACTERIZATION OF Cd-Zn-Te FILMS

A. *Optical Transmission*

The optical transmission measurements on Cd-Zn-Te films deposited at different Zn source temperatures are shown in the Fig. 2.

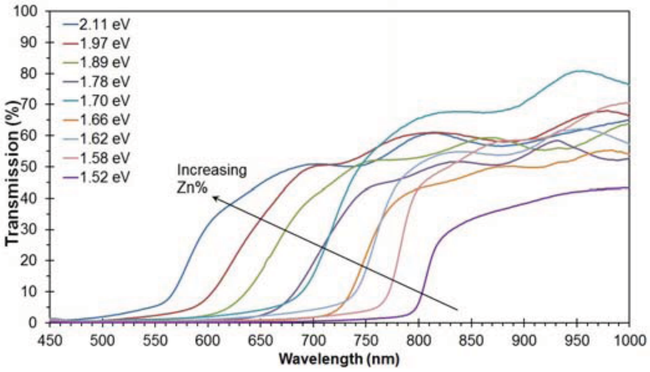
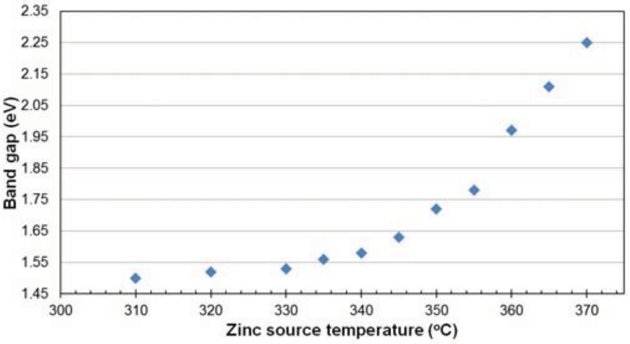


Fig. 2. Transmission measurements on the Cd-Zn-Te films with varying Zn composition.

At temperatures near 320^{o}C, the band gap of the films is close to the band gap of CdTe. This suggests that zinc vapor flux generated at these temperatures is lower and incorporation of zinc in CdTe is low. With the increase in the source temperature of zinc, the shift in the transmission edge towards the shorter wavelength occurs due to alloying of Cd-Zn-Te. The plot of band gap vs Zn source temperature (Fig. 3) demonstrates controllable alloying of Cd-Zn-Te.

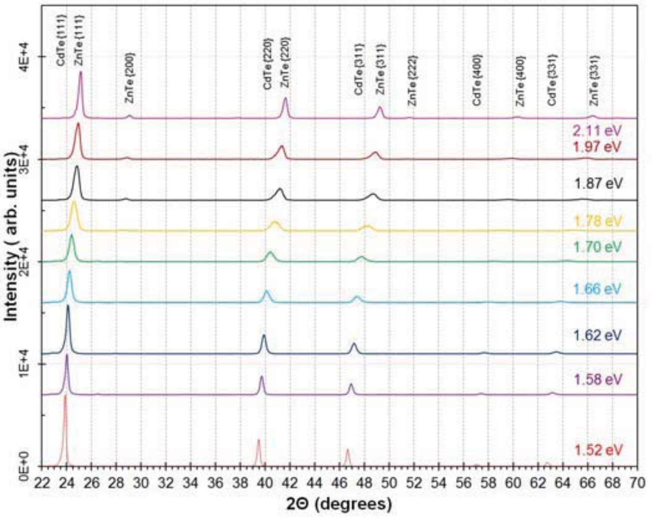
Fig. 3. Band gap of deposited Cd-Zn-Te films vs. Zn source temperature in the co-sublimation source.



B. *GAXRD*

To allow for a better comparison, the diffraction patterns for all Cd-Zn-Te films were obtained with the same scan speed of the detector and counts of incident X–rays (Fig. 4).

Fig. 4. GAXRD shows shift in the diffracted peaks from CdTe to ZnTe with increasing zinc source temperature.



The location of the diffracted peaks generated from the sample fabricated with Zn source temperature at 320^{o}C exhibited a pattern close to CdTe (ICDD#00-015-0770). With increasing Zn source temperature, the diffracted peaks shifted towards the higher angles indicating formation of Cd-Zn-Te alloy. The film with band gap 2.11 eV had diffracted peaks close to ZnTe (ICDD #00-015-847). In all the films, the first peak had the highest intensity indicating that preferred orientation along {111}. The lattice parameters were calculated based on the peak locations and compared with the data in literature (Fig. 5).

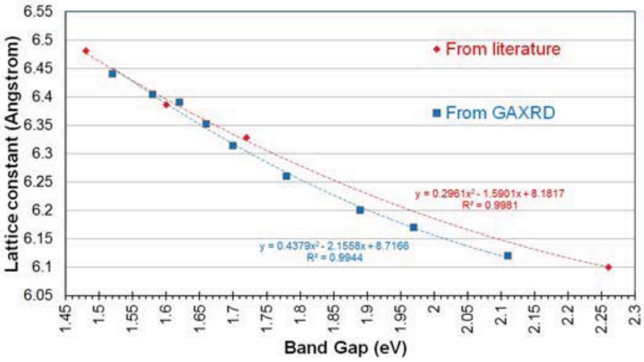


Fig. 5. Lattice parameter calculated from the GAXRD vs. Band gap of the deposited Cd-Zn-Te films estimated from the transmission and compared to the values found in the literature [20].

IV. Device Performance

A. External Quantum Efficiency

The EQE for Cd-Zn-Te with a band gap of 1.72 eV covered with Al_2O_3 as a barrier did not show any current generation from photons of a lower energy than as-deposited band gap (Fig. 6). This indicates that the composition of Cd-Zn-Te film is maintained after the $CdCl_2$ treatment and Al_2O_3 is an effective barrier to prevent loss of zinc from the back surface of Cd-Zn-Te when processed in this manner.

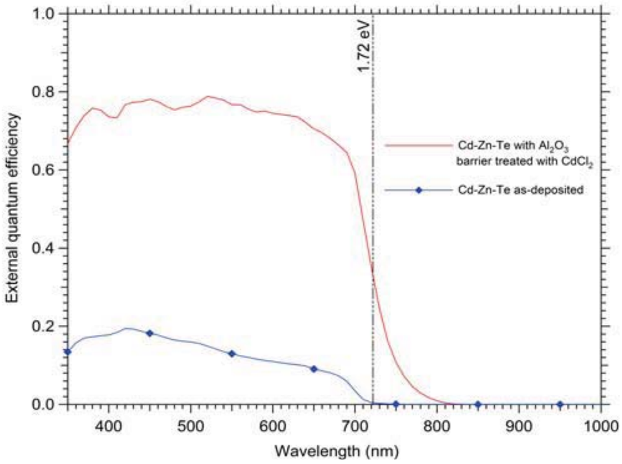


Fig. 6. EQE comparison of sample treated with $CdCl_2$ having Al_2O_3 as a barrier (etched after $CdCl_2$) and as-deposited Cd-Zn-Te.

B. External Quantum Efficiency under Biasing Conditions

As shown in the Fig. 7, EQE measurements were taken with the device under different applied biases. The depletion width would have changed but there was no current generation beyond 1.72 eV. This confirmed that there were no significant compositional changes in the Cd-Zn-Te absorber after the $CdCl_2$treatment.

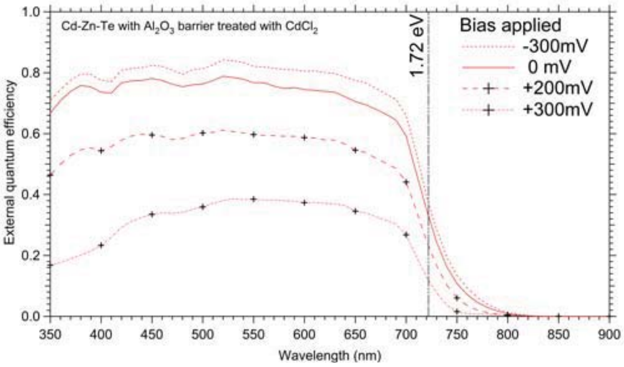


Fig. 7. EQE under applied bias on Cd-Zn-Te sample with Al_2O_3 barrier treated with $CdCl_2$.

V. Summary of the Work

In this work, Cd-Zn-Te films with different band gaps were deposited by using co-sublimation of CdTe and Zn. The composition of the films was varied by controlling the source temperature of zinc source. The shift in the transmission to shorter wavelength and decrease in the lattice constant with increase in the zinc incorporation was observed. Alumina on the back of Cd-Zn-Te was used as a barrier to minimize zinc loss during the $CdCl_2$ treatment. After etching the alumina, fabricated devices showed no loss of zinc in the EQE measurements.

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