Optik 160 (2018) 307–321

Contents lists available at ScienceDirect

Optik

journal homepage: www.elsevier.de/ijleo

Original research article

Effect of $CdCl_2$ heat treatment in $(Ar + O_2)$ atmosphere on structural and optical properties of CdTe thin films

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ARTICLE INFO

Article history:
Received 11 December 2017
Received in revised form 26 January 2018
Accepted 28 January 2018

Keywords:
CdTe thin films
$CdCl_2$ heat treatment
X-ray diffraction
Field emission scanning electron microscope
Optical energy gap

ABSTRACT

Cadmium telluride (CdTe) thin films were deposited by thermal evaporation method under base pressure 2×10^{-5} mbar on corning glass substrate. In this work, we study the effect of cadmium chloride ($CdCl_2$) heat treatment in argon and oxygen $(Ar + O_2)$ atmosphere on the structural, morphological and optical properties of CdTe thin films to achieve high quality thin film absorber layer for solar cells applications. The structural characteristics were studied by X-ray diffraction (XRD). The microstructure parameters of the films such as average grain size (D_{avg}), average lattice strain (ε_{avg}) and dislocation density (ρ_D) have been calculated via XRD line broadening analysis. XRD investigation revealed that, the samples show polycrystalline nature pronounced with cubic zinc blende structure with a strong preferentially (1 1 1) texture orientation. It has been found that the crystallinity of the films enhanced during $(Ar + O_2)$ annealing and $CdCl_2$ heat treatment. The surface morphology of CdTe thin films was investigated by field emission scanning electron microscope (FE-SEM). XRD and FE-SEM results of $CdCl_2$ treated films showed recrystallization and progressive increase in grain size. The optical properties of all samples were estimated using UV–vis–near-infrared (NIR) spectrophotometer. The Swanepoel envelope method has been employed to evaluate the various optical parameters of CdTe films such as refractive index and film thickness. The as-deposited films have a relatively high value of refractive index of 2.54, in contrast the $CdCl_2$ treated films have a relatively low value of 2.1 in the whole wavelength range. The optical energy gap values slightly decrease from 1.56 eV for as-deposited films up to 1.54 eV for $CdCl_2$ heat treated films. $CdCl_2$ heat treatment in $(Ar + O_2)$ atmosphere is found to be a promising method to improve the physical properties of CdTe thin film solar cells.

1. Introduction

The II–VI semiconductor compounds, i.e., cadmium telluride (CdTe) has been in the focus of comprehensive research due to their possible utilization in many applications such as Opto-electronic devices [1,2], photovoltaic cells [3], laser windows material [4,5], gamma rays and X-ray detectors [6,7], photoconductive devices [8], and light emitting diodes [9]. The main fundamental characteristics of CdTe are: perfect direct band gap around 1.45 eV at room temperature (RT), which is the optimum value for solar cell devices [10], it is cheap and inordinately steady during the application processing, resulting

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https://doi.org/10.1016/j.ijleo.2018.01.112

in powerful interests and quick evolution of CdTe-based solar cells devices in recent years [11], large optical absorption coefficient (>10^4 cm^{-1}) which means that around 90% of incident sunlight in the visible range can be absorbed by only a few micrometers of CdTe thin films. CdTe is one of the most suitable candidates as absorber layer for CdTe/CdS solar cells devices [12,13]. Solar cells which formed from CdTe/CdS systems are one of the expected candidates for prevalent commercial success in solar energy transformation. On the other hand, CdTe can be formed in both n-type and p-type conductivity, therefore, CdTe is useful for homojunction and heterojunction organization.

CdTe thin film has been prepared by many different techniques like, thermal evaporation [14], electron beam evaporation [15], RF sputtering [16], sol–gel spin coating [17], close spaced sublimation (CSS) [18,19], pulsed laser deposition (PLD) [20], electrodeposition [21,22], metalorganic chemical vapor deposition (MOCVD) [23], spray pyrolysis deposition (SPD) [24], screen printing [25], molecular beam epitaxy (MBE) [26] and chemicals deposition techniques including chemical bath deposition (CBD) [27]. The thermal evaporation is the most widely method for preparation of thin films because of its easy to use, scalability and reproducibility [28,29]. Furthermore, the deposition rate is high which can be controlled easily and damage to the substrate during deposition can be minimized.

Several studies have reported on the physical properties of CdTe thin films. However, the effect of $CdCl_2$ heat treatment on the optical and structural properties of CdTe thin films has not been fully studied yet. Generally, the as-deposited films would have many undesirable characteristics that affect the competence of the device execution, such as small grains, low crystallinity and many grain boundaries which lead to high electrical resistivity. The existence of Cl atoms could diffuse into the grain boundary of CdTe thin films during crystal growth which causes improve the recrystallization, the grain growth, and electronic properties of CdTe thin films [30,31]. In fact, the main key for enhancing the efficiency of the thin film solar cell is heat treatment by $CdCl_2$ on the top of the CdTe thin films (300–400 nm) with annealing temperature in the range 350–450 °C for 10–60 in air or inert gas under atmospheric conditions. Several researchers have been studied this treatment to improve the efficiency of solar cell thin film; however, a full comprehension of that treatment has not been completed yet and remain a subject of discussion.

The major objective of this study was to investigate the effects of $CdCl_2$ heat treatment in ($Ar + O_2$) atmosphere on physical properties of thermally evaporated CdTe thin films and compared with ($Ar + O_2$) annealing process. This study has been carried out by X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM) and UV–vis–near-infrared (NIR) spectrophotometer. The structural, morphological and optical properties on these films are reported in this paper.

2. Preparation and examination of CdTe thin films

2.1. Deposition technique

CdTe thin films were prepared by thermal vacuum evaporation technique (Edward's high vacuum unit model AUTO 306) using a stoichiometric CdTe powder (99.999%) from Sigma Aldrich as a source material. The CdTe thin films were deposited onto corning glass substrates (1 cm × 1 cm × 0.1 cm). The glass substrates were cleaned in an ultrasonic bath in deionized water, acetone and ethanol and dried using an argon gas flow. The CdTe films were deposited with a thickness between 1100 and1200 nm at room temperature with a base pressure of 2×10^{-5} mbar. The deposition rate and film thickness during the deposition process can be controlled by the digital film thickness monitor (INFICON SQM-160). The deposition rate was varied in the range of (2–3) Å/s. The chamber pressure was approximately constant at 5×10^{-5} mbar and 2×10^{-5} mbar at room temperature (RT) in the beginning and end of film deposition respectively.

2.2. $CdCl_2$ heat treatment and ($Ar + O_2$) annealing procedure

The heat treatment in ($Ar + O_2$) atmosphere with the presence of $CdCl_2$ was carried out inside a furnace tube model Kejia to improve the optical and structural properties of the CdTe thin films. On the other hand, annealing in ($Ar + O_2$) atmosphere is preferred to air ambient when preparing efficient CdTe solar cell to avoid the impurities from air which can affect the film structure. Fig. 1 summarized the heat treatment procedure. The heat treatment process can be summarized as:

(a) $CdCl_2$ layer of thickness about 150 nm has been deposited on the top of the as-deposited CdTe thin films by thermal evaporation technique.
(b) The achieve of thermal annealing was carried out by the temperature sequence at 400 °C for 15 min, 450° for 15 min and finally at 480 °C for 10 min.
(c) During heat treatment process the gasses of Ar and O_2 were flowing in the furnace tube by rate of 8 sccm.
(d) The samples were kept in the furnace tube until their gradual cooling to room temperature is achieved, which takes around 3 h.
(e) The ($Ar + O_2$) annealing experimental was done under the same conditions (i.e., time, temperature, gas flow) without the presence of $CdCl_2$.