International Journal of New Horizons in Physics

http://dx.doi.org/10.18576/ijnhp/100102

Effect of heat treatment in structural and optical properties of 1 µ of Cu/CdTe thick film

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Received: 2 Aug. 2022, Revised: 4 Dec. 2022, Accepted: 8 Dec. 2022

Abstract: In the current study, 1 m thick Cadmium Telluride (CdTe) coatings on glass substrate were created using thermal evaporation procedures (at temperature about 150 ºC). The produced films were doped by ion exchange with Cu by submerging them in a solution of $Cu(NO_3)_2$ (1g/1000ml) for 30 minutes. Additionally, for the diffusion of the dopant Cu content, the doped films were annealed in vacuum for 60 minutes at various temperatures (RT, 100, 200, 300, 400, and 500 ºC). The initial treatment mix was defined by the (EDAX). Cu was present in an average concentration of 10±2% at.% throughout all treated films, which was essentially constant. The structural characteristics for the untreated and treated films (lattice strain and crystallite size) were calculated using the XRD pattern. Swanepoel's method was used to determine the film thickness and refractive index of films. Experimental observations of transmission and reflection in a high absorption region were used to calculate the films' energy gap. The transmittance and reflection spectrum in the high absorption area were used to measure the optical band gap. The conceivable transition in these as-deposited and as-treated films is found to permit a direct transition with a band gap reduction from 1.50 at room temperature to 1.29 at 300 ºC with a rise in temperature. After 300, the energy gap reverses its direction and increases. Crystallize size and lattice strain changes can both be used to explain changes in optical characteristics. For optoelectronic devices, Cu/CdTe films are recommended due to the optical constants' turnability.

Keywords: Heat treatment; Cadmium Telluride (CdTe); thermal evaporation; structural and optical properties; Cu/CdTe thick film

1 Introduction

Cadmium telluride is an important substance that is used in many products, such as photovoltaic cells, photorefractive systems, and electro-optic modulators [1]. CdTe films exhibit both n- and p-type electrical conductivity in the variety of detectors that operate in the infrared, ultraviolet, X-ray, and gamma ray spectrums [2], making them useful for diodes and transistors [3]. CdTe has a direct optical energy gap of 1.5 eV at room temperature, which is appropriate for the junctional performance of solar cells [4, 5]. With a 16.8% efficiency, CdTe/CdS solar cells were built by Brit and Freckids [6]. The ability to fabricate these materials using a range of techniques is made possible by the low evaporation temperature of CdTe polycrystalline films [7–13]. The close-spaced sublimation technique is one of many that has produced good outcomes (CSS). The CSS method can be used forever with various chemical systems that are sublimating continually. It provides compensation in the form of an easy-to-use deposition method and highly effective transport that both operate at low vacuum and moderate temperatures [14]. Both the Group I elements Silver (Ag) and Copper (Cu) are mentioned as replacement acceptors in CdTe. Cu as a p-dopant is the most popular way to dope thin CdTe polycristalline films [15]. Class II-VI semiconductor CdTe has a high light absorption coefficient and a medium band gap of 1.45 eV. (over 104 cm1 in the optical range).

Numerous investigations have been contaminated with CdTe film constituents including Sb, Ag, Cd, Te, etc. [16–19]. Cu doping, on the other hand, presents difficulties for CdTe polycrystalline thin films [20]. It is projected to be used for light gathering and is considered a desirable material for solar cell applications [21, 22]. It can be difficult to produce a low and reliable ohmic contact with CdTe (low resistance of CdTe/back contact electrode), which is one of the primary problems with CdTe solar cells [23]. in order to create a low resistance CdTe contact. Cu is the most often used metal to induce acceptor

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states in CdTe at concentrations up to around 1019 cm-3 [24, 25]. Studies show that Cu can either manifest as interstitial flaws or substitutional faults (CuCd) (Cui). After heat treatment, Cui can move quickly through the CdTe film, leading Cu to concentrate at the pn junction's interface and cause an N-type compensation brought on by Cu+, which reduces device performance. CuCd is a deeper acceptor level (0.15-0.34 eV), whereas Cui is a shallow donor (0.01 eV) [26]. It has been found that during heat treatment, the copper interstitial atoms (Cui) can travel swiftly in the CdTe film, leading Cu to accumulate at the pn junction interface and produce an N-type compensation brought on by Cu+, which reduces device performance [27, 28]. This suggests that the instability of CdTe/CdS solar cells is also believed to be caused by the diffusion of Cu in CdTe. Therefore, it is vital to control the efficient doping of copper through heat treatment in order to generate stable and functional thin-film solar cells. Cu will have a high solubility and diffusion in compounds containing II-VI at temperatures of several hundred degrees Celsius. Copper serves a variety of purposes in gadgets like solar cells. By increasing the p-doping of CdTe close to the back contact interface, it causes solar degradation in addition to aiding in the creation of a good ohmic contact. The manufactured CdTe films are exposed to an ion exchange method that diffuses Cu into CdTe thin films by immersing them in a solution of Cu(NO3)2 for 30 minutes. They were also annealed in a vacuum to enhance the diffusion of Cu into the implanted films. Researchers have studied how annealing impacts the optical constants and microstructure parameters of CdTe films containing Cu implants in order to better understand these effects. By adjusting the Cu diffusion in CdTe through thermal annealing, the efficiency of the solar cell can be changed.

2 Experimental

Target material CdTe powder with a purity of 99.99 percent was bought from Aldrich Chemical (USA). A Denton Vacuum Coating Unit (DV 502 A) and vacuum of around 10^{-6} Pa were used to deposit 1000 nm thick CdTe films on a glass substrate that had been ultrasonically cleaned and kept at temperature (150 ^{o}C) from a quartz crucible heated by resistance. The rate of deposition and thickness of the thick film were controlled throughout deposition using a quartz-crystal (DTM 100) monitor. The rate of deposition was kept constant at 2 nm/s during sample preparation. CdTe films were then immersed in a solution of Cu $(NO_3)_2$ (1g/1000 ml) for an additional 30 minutes. These films were then compressed to dry and cleaned in distillation water. Additionally, the heat treatment (annealing) was carried out in vacuum for 30 min. at various annealing temperatures (RT, 100, 200, 300, 400, and 500^{o}C) for the dispersion of dopant Cu material into CdTe thick films. In order to evaluate the morphology of the treated films, an energy dispersive X-ray spectrometer unit (EDX) was interfaced with a scanning electron microscope, SEM (Japan, JEOL-JSM-6360LA), and used to analyse the elementary composition of the treated films. By expending an XRD analysis (Philips-X-ray diffractometry (1710) and a Cu K radiation target ($\lambda = 0.15418$ nm), the structure of the ordered films was examined. When collecting the intensity data, a small interval phase scanning mode ($2\theta = 0.02^{o}$) was used. A double-beam spectrophotometer (Shimadzu UV-2101 in conjunction with a computer) was used to measure both reflection and transmission at perpendicular light incidence and over the wavelength array of 400 to 2500 nm. Without a glass substrate in the position beam, to calculate the refractive index and film thickness of CdTe thin films, the acquired transmittance spectra were used.

3. Results and discussion

3.1 Elemental composition analysis

The stoichiometric composition of CdTe and the configuration of surrounded thick films of CdTe:Cu are presented in Figs. 1(a) and 1(b), respectively, using EDXS. The average concentration of Cu was 9.86 at. %, which was nearly constant throughout all treated films.

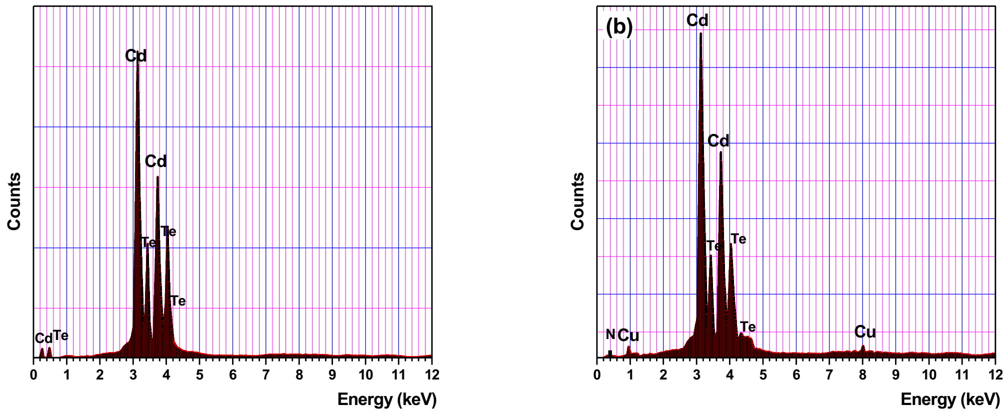

Fig. 1: EDAX for (a) as deposited CdTe and (b) treated CdTe:Cu thin film at 500^{o}C.

3.2 X-ray diffraction analysis

A technique for characterising crystalline materials is Rietveld refinement [29]. The reflections (intensity of the peaks) at specific points in the XRD pattern of the CdTe powder samples were distinctive. A variety of characteristics of the material structure can be inferred from the height, width and position of these reflections. Until a theoretical line profile fits the observed profile, the Rietveld method uses a minimal square approach to modify the profile. The diffraction peaks of the as-deposited and entrenched films from the cupper blend of CdTe (JCPDS Data File: 37-1027-cubic) are shown in Fig. 2, with their preferred orientation along the (111) plane. The main physical characteristics of these trends are the same, however there are only minor variations in the peak duration. Sharp diffraction peaks were found for the values of diffraction angle 2 θ= 23.99, 39.73, and 46.86, respectively, corresponding to (111), (220), and (311) orientated planes, and this was consistent with the literature [30-32]. Fig. 2. Additionally shows that when the temperature at which CdTe:Cu films are annealed and the diffracted strength of the (111) plane rise, Cu doping significantly increases the crystallisation efficiency of deposited films. The instrumentation factor and the structure factor, which depend on the strain of the lattice and the size of the crystal, are responsible for the peak broadening. The Scherrer and William-Hall equations were used to calculate the crystallite size (D) and lattice strain (e).

$$D_v = \frac{k\lambda}{\beta\cos(\theta)}$$

and

$$\varepsilon = \frac{\beta}{4\tan(\theta)}$$

where β is the structural width, that given by

$$\beta = \sqrt{\beta_{obs}^2 - \beta_{std}^2}$$

and which corresponds to the discrepancy between the film's width and the width of a normal silicon wafer.

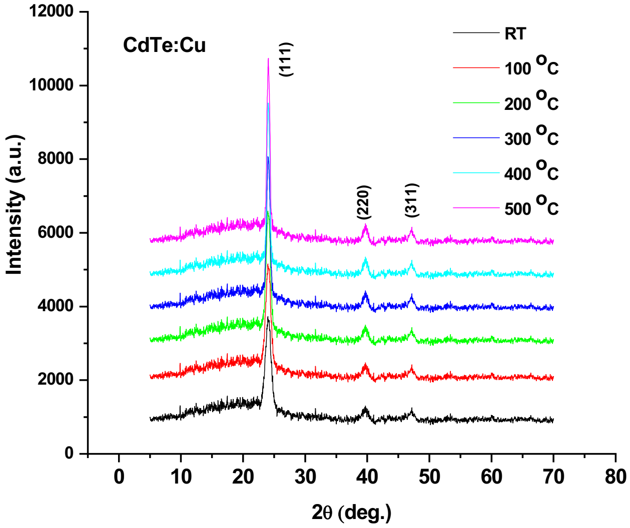

Fig. 2: X-ray diffraction pattern of CdTe:Cu thin films annealed at various temperatures.

The two parameters (crystallite size D and lattice strain e) of the deposited and annealed CdTe thick films are shown in Figs. 3 and 4. It is demonstrated that as annealing temperature is raised, the average size of the crystallite increases as a sigminoidal behaviour while the strain on the lattice reduces as an anti-sigminoidal behaviour. This indicates that as crystallite size increased, it did so initially at a smaller rate before progressively increasing to a larger value at 500 °C for annealing. The observed behaviour of microstrain might be related to a growth in crystallite size. A reduction in the concentration of lattice defects is also reflected by a decrease in lattice strain, which may be caused by a narrowing of the lattice with higher annealing temperatures.

3.3 Optical parameters

Both T(λ) and R(λ) are shown vs wavelength, in Fig. 5. An outstanding quality and similarity of the treated CdTe:Cu films were confirmed by the appearance of interference fringes, the maximum of transmission and minimum of transmission in the T(λ) spectrum. Swanepoel's envelope approach, which was used to compute the index of refraction, n, proved successful [30-32]. The T(λ) spectrum of a thick CdTe film with d = 1000 nm is shown in Fig. 6. The following relationship can be used to compute the n value using this envelope method at a given wavelength.

$$s = \frac{1}{T_s} + \sqrt{\left(\frac{1}{T_s} - 1\right)}$$

$$T_{M_j} = T_0 + A_1 e^{-\frac{\lambda_j}{t_1}} + A_2 e^{-\frac{\lambda_j}{t_2}}$$

$$T_{m_j} = T_0 + A_1 e^{-\frac{\lambda_j}{t_1}} + A_2 e^{-\frac{\lambda_j}{t_2}}$$

Here, the maximum and lowest transmittances are denoted by TM and Tm at a given.

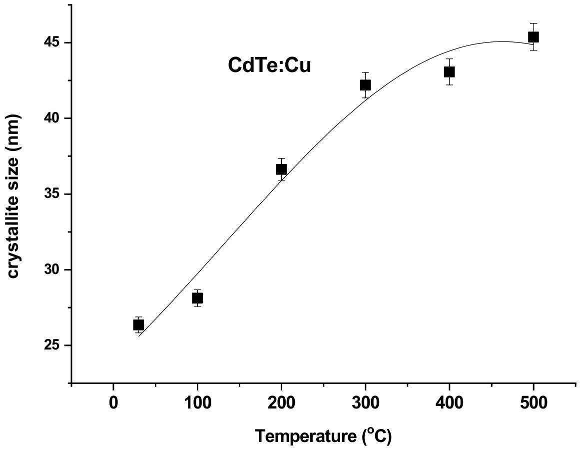

Fig. 3: Crystallite size of annealed CdTe:Cu thin films

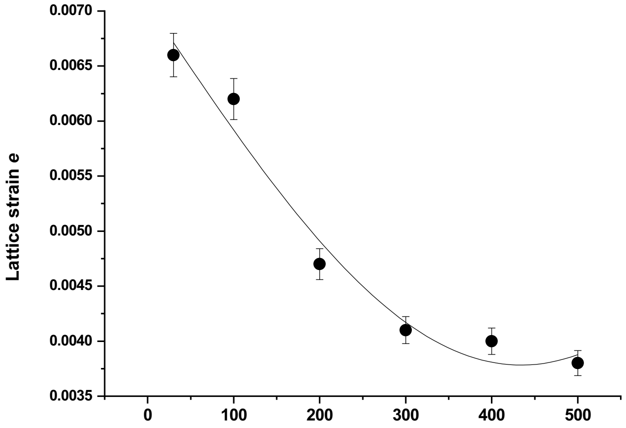

Fig. 4: Lattice strain in thin CdTe:Cu films after annealing.

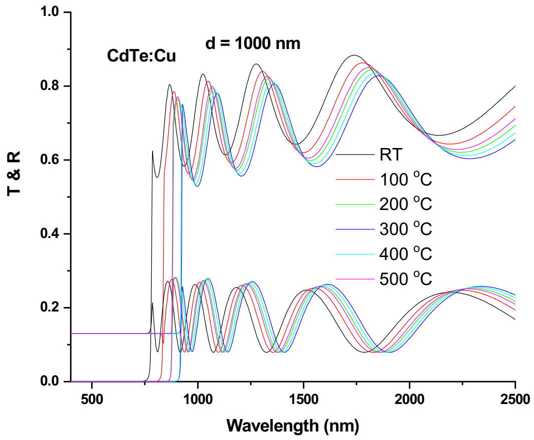

Fig. 5: The Reflection and Transmission spectrum of CdTe:Cu films at different annealing temperature.

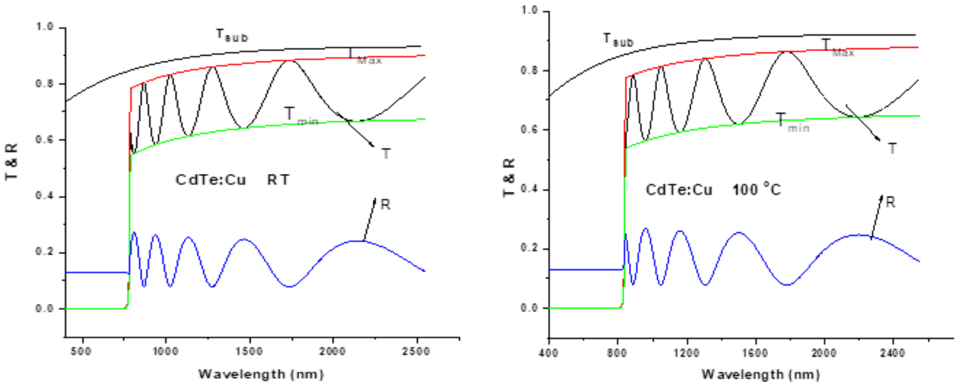

Fig. 6: The Swanepoel's envelope method of *T* spectra showing the interference fringes maxima and minima.

The *n* values, which were calculated using eq:

$$n_1 = \sqrt{N + \sqrt{N^2 - s^2}}$$

where

$$N = 2s\left[\frac{T_{M_j} - T_{m_j}}{T_{M_j} T_{m_j}}\right] + \left[\frac{s^2+1}{2}\right]$$

are shown in Fig. 7. Additionally, nl and n2 are the refractive indices at two nearby maxima (or minima) at λ1 and λ2, so the expression results in the following film thickness:

$$d_1 = \frac{\lambda_{e1}\lambda_{e2}}{2[\lambda_{e1}n_{e2} - \lambda_{e2}n_{e1}]}$$

According to Fig. 7, the refractive index value increases until it reaches a temperature of 300 0C, after which it starts to decline as the temperature rises. The absorption coefficient can be calculated using the following expression (12, 13) in agreater absorption area for both T(λ) and R(λ):

$$\alpha = \frac{1}{d}\ln\left[\frac{(1-R)^2 + \sqrt{\{(1-R)^4 + 4R^2T^2\}}}{2T}\right]$$

where d is the film's thickness. The relationship between "(hν) on photon energy, hν" and "annealing temperature" is depicted in Fig. 8. The strong absorption edge of pure semiconducting substances is well recognised [33, 34]. With an increase in annealing temperature from RT to 500 °C, the absorption edge became sharper and shifted to higher wavelengths. It is understood that for a direct transition from valance band to conduction band, the value is designated in the vicinity of the fundamental absorption edge [15]. Fig. 9 shows the best fit of (αhν)2 vs. hν for differs annealing temperature of Cu doped CdTe film. You can think of the direct optical band gap as the capture of (hν)2 versus. (hν) at (α hν)2 = 0. The E_g^{opt} resulting for each film is shown in Fig. 10. In terms of the T and R spectra, the optical energy gap in the high area of the absorption was calculated. With an increase in the annealing temperature, the energy gap falls from 1.50 to 1.37 eV. The addition of Cu ions in the lattice, which causes the rise in the bandgap acceptor levels, may be the cause of the decrease in the energy gap. The bandgap is reduced as a result of the valence band expanding into the forbidden region as a result of the acceptor rates descending and joining together [35, 36].

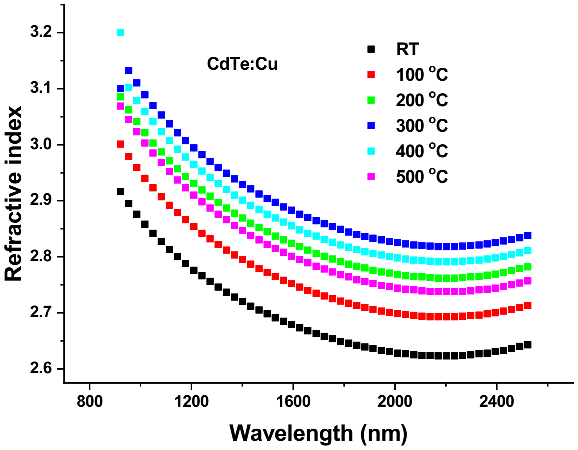

Fig. 7: The refractive index vs. wavelength of CdTe:Cu films at different annealing temperature.

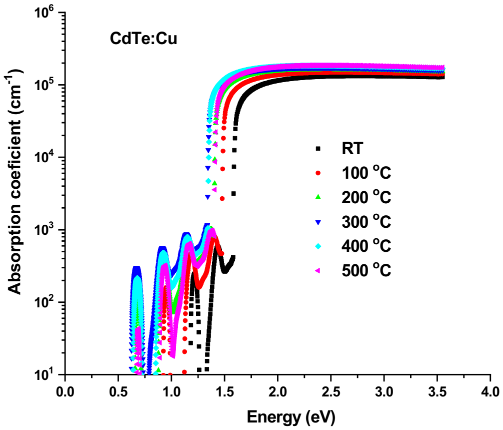

Fig. 8: Absorption coefficient (α) aganist incident photon energy ($h\nu$) for CdTe:Cu films at various annealing temperature.

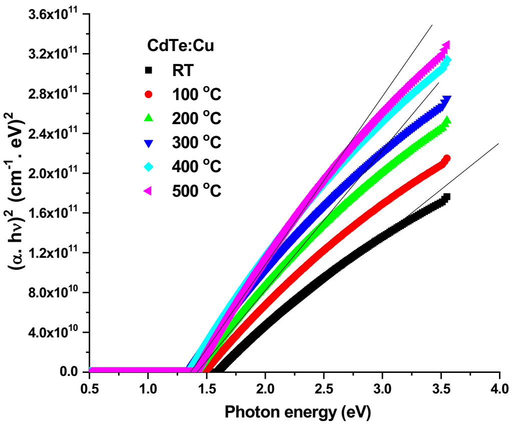

Fig. 9: $(\alpha h\nu)^2$ as a function of $(h\nu)$ for CdTe:Cu films at various annealing temperature

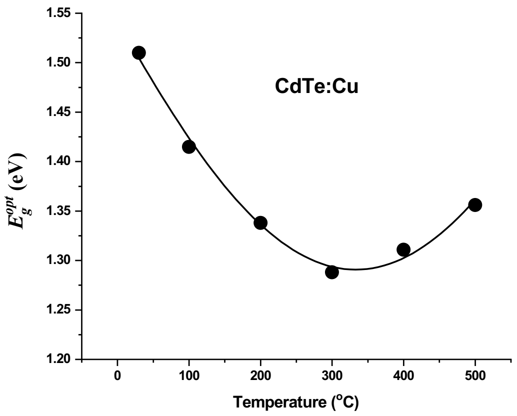

Fig. 10: Values of energy gap as a function of annealing temperature for CdTe:Cu films.

4 Conclusions

CdTe films that were doped with Cu using the ion exchange method were prepared using thermal evaporation procedures. The doped films were treated (annealed) in vacuum for 30 min. at a variety of annealing temperatures (RT, 100, 200, 300, 400, and 500 oC). Using the envelope the transmission method, the refractive index, n, and film thickness, d, were both determined. The n value rises as the annealing temperature rises. Scherrer and Welson equations were used to compute the crystallite size and lattice strain. Practically speaking, the strain on the lattice reduces as the annealing temperature is raised while the average size of the crystallite grows. In terms of the T and R spectra, the optical energy gap in the high area of the absorption was calculated. With an increase in annealing temperature, the energy gap falls from 1.50 at room temperature to 1.29 at 300 ^{o}C. For as deposited and treated CdTe, the dielectric constants (1, 2) and energy loss functions (VELF, SELF) were calculated and explained in terms of the growing annealing temperature. From 1.50 at (RT) to 1.29 at (300 ^{o}C) eV, but as temperature keeps rising after 300, the energy gap reverses direction and widens. The decrease in crystalline size till 300 ^{o}C and the influence of rising lattice strain generates an inflection of energy gap can be used to explain the change in optical characteristics.

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