PAPER • OPEN ACCESS

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To cite this article: N M D Putra et al 2019 J. Phys.: Conf. Ser. 1321 022018

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Absorber performation of CdTe/CdTe:Cu thins films based from crystal phase and microstructures

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1321 (2019) 022018

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Abstract. It has been successfully grown thin film CdTe, CdTe:Cu (2%) and CdTe:Cu (15%) using DC Magnetron Sputtering method. Sample preparation was performed with different temperature and plasma power parameters above the ITO (Indium Tin Oxide) substrates. Then sample a thin film on annealing for 20 minutes. The addition of Cu doping causes the film polycrystalline structure to change from zincblende (cubic) to wurtzite (hexagonal) crystal phase. The optical transformation of CdTe as absorber is indicated parameter by the Eg = 1.48 eV or $\alpha = 7,348 \times 10^4$ cm⁻¹ corresponding to the CdTe:Cu (2%) thin film sample with optimum crystal size and high lattice parameters.

1. Introduction

CdTe thin film solar cells are one of the most promising for photovoltaic energy conversion. The maximum theoretical efficiency for CdTe/CdS solar cells, on standard spectrums, is around 30% [1].

In accordance with the growth carried out, CdTe thin films can show n-type or p-type electrical conductivity. It is known that excess cadmium (Cd) produces n-type conductivity while excess telluride (Te) produces p-type [2]. In this system the p-type CdTe thin film plays a role as an absorber layer [3].

One of the limitation to improve efficiency is the difference between the crystal structure of CdTe and CdS, each of which is cubic and hexagonal, because the large defect meeting is generated by the interface [4]. The way to reduce this is to grow two layers with the same phase crystals. Because the stable phase of CdS is hexagonal, it is very important to obtain CdTe in the hexagonal phase.

The high efficiency performance of CdTe thin film solar cells in many Researchers shows Cu doping contributions which were originally introduced as back contact [5]. Addition of Cu in CdTe/CdS solar cells can affect and replace the Cd site [6] so that it can change the structure conditions of CdTe and CdS. In this study, the effect of Cu doping on CdTe performance as an absorber will be examined in terms of the crystal phase and its microstructure.

2. Methods

Undoped and Cu-doped CdTe films were grown on Indium Tin Oxide (ITO) substrates by modified DC Magnetron Sputtering. The target is made with a pressing system with a hydraulic pump into a pellet measuring 2 cm in diameter. The materials employed were powders of CdTe and Cu_2Te with a purity of 99.99%. The powders were mixed by ball milling. Films were grown at substrate temperatures 250 and 325 °C. Four samples were prepared and studied: two Cu-doped CdTe films and two undoped CdTe films. The background pressure in the deposition chamber was 10^{-4} Torr and 43 W plasma power. The vacuum in the chamber was maintained during the growth. The growth time was 2.5 hours. The crystalline structure was determined by X-ray diffraction (XRD) with a Siemens D5000 diffractometer, using the Cu-K α line. The surface morphology and grain size of the films were observed by scanning

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electron microscopy (SEM) using a FESEM-Carl Zeiss Auriga. The transmittance spectra were obtained using an UV-Vis Perkin Elmer Lambda 25 spectrophotometer.

3. Result and Discussion

Morphological imagery of SEM thin films CdTe and CdTe:Cu (15%) grown at a substrate temperature of 250 °C is shown in Figure 1(a) -1(b). While the morphological image of SEM thin films CdTe and CdTe:Cu (2%) grown at substrate temperature 325 °C is shown in figure 1(c) -1(d). In the picture it is shown that the CdTe films shows uneven grains. Addition of Cu causes the resulting grains to be evener. This is related to the role of Cu in CdTe as an interstitial ion (Cu⁺) which will fill the vacancy of Cd (Cd vacancy) [7].



Figure 1. Morphological images of SEM thin films (a) CdTe and (b) CdTe:Cu(15%) grown at a substrate temperature of 250 °C; Morphological image of SEM thin film (c) CdTe and (d) CdTe:Cu(2%) grown at 325 °C substrate temperature.



Figure 2. Results of XRD characterization of thin films of CdTe and CdTe:Cu(15%) grown at a substrate temperature of 250 °C.



Figure 3. Results of XRD characterization of CdTe and CdTe thin films: Cu(2%) grown at 325 °C substrate temperature.

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In Figure 2 shows that in both XRD spectra the highest peaks of thin films CdTe and CdTe:Cu are oriented at 39.26° which corresponds to the hexagonal phase and diffraction plane (110)H [8]. However, in the XRD spectrum CdTe found several other peaks, namely at 76.12° orientation which corresponds to the cubic phase and diffraction plane (511)C [9]. Whereas the XRD CdTe:Cu spectrum has several additional peaks, which are not possessed by CdTe, ie at orientations of 48.30° , 54.92° and 67.23° , each of which corresponds to the diffraction (201)H, (202)H and (105)H fields. Based on this, Cu(15%) doping on CdTe grown at 250° substrate temperature has succeeded in changing the CdTe thin film from the cubic phase to the hexagonal phase. However, the addition of Cu doping causes a lot of visible orientation of Cu₂Te. This is due to Cu's high doping concentration 15%. The addition of Cu doping also causes the peak of ITO in orientation (400) to no longer be seen. This is because the thin film CdTe:Cu(15%) has a morphology that is relatively more even than the CdTe film, although the peak ITO in orientation (700) is still visible.

In Figure 3 the XRD characterization of thin films of CdTe and CdTe:Cu(2%) shows that the two films have the highest peak at 28.93° orientation which corresponds to the hexagonal phase structure and diffraction plane (101)H. From the JCPDS data [8], both films also have a hexagonal structure, but the quality of the peak intensity of the fields (100)H and (101)H in the diffraction spectrum of XRD CdTe:Cu(2%) is higher than in the XRD CdTe spectrum. Thin films of CdTe and CdTe:Cu(2%) were grown at 325° when compared with thin films of CdTe and CdTe:Cu(15%) grown at 250 °C (figure 2), had better quality, ie not has ITO peak because it has a relatively flat morphology (figure 1(c) and 1(d)). Likewise, no Cu₂Te orientation peaks were found because Cu doping concentrations were low (2%).

Table 1. Variation of microstructure parameters for CdTe, CdTe:Cu(15%) and CdTe:Cu(2%) preparedat temperatures of 250 °C and 325 °C.

Sample	σ	a (A)	D (nm)	δ (x10 ¹¹ cm ⁻²)	ε (x10 ⁻⁴)
CdTe - 250	0.424	6.487	28.3	1.224	2.950
CdTe:Cu(15%) -250	0.652	6.491	28.6	1.404	6.125
CdTe - 325	0.423	6.485	29.5	1.083	2.575
CdTe:Cu(2%) - 325	0.357	6.485	30.4	1.148	1.938

Microstructure analysis is performed including calculation: degree of orientation (σ) [10], lattice parameter (a) [11], crystallite size (D) [12], dislocation density (δ) [13,14] and micro strain (ϵ) [14,15]. Table 1 shows the results of microstructure analysis for CdTe, CdTe:Cu(15%) and CdTe:Cu(2%) prepared at temperatures of 250 °C and 325 °C. Both CdTe thin films without Cu doping at temperatures of 250 °C and 325 °C revealed similar microstructure parameters. Only the dislocation density (δ) and micro strain (ϵ) parameters of the CdTe thin film grown at 325 °C have a lower value. Temperature effects have succeeded in reducing the possibility of higher crystal defects. In another part, the CdTe:Cu thin film (15%) has a microstructure parameter value that is greater than CdTe:Cu(2%) except in the parameter crystallite size (D). High values of degree of orientation (σ), lattice parameters (a), dislocation density (δ) and micro strains (ϵ) due to the large Cu doping effect. Excessive Cu Doping tends to worsen crystal quality.

The absorbance graph for the wavelength of the thin film CdTe and CdTe:Cu(15%) is shown in figure 4(a). From the graph, it can be seen that the CdTe thin film is only able to absorb light at a wavelength range of 454 nm down while the thin film CdTe:Cu(15%) is only able to absorb light in the wavelength range 439 nm down. Both films have not shown good characteristics for solar cell maker materials. F. de Moure-Flores *et al.* [3] suggested that the CdTe thin film which is good for solar cell applications is the CdTe thin film which is able to absorb almost the entire visible light spectrum, which is at a wavelength range of 800 nm and below.

In Figure 4(b) it can be seen that both films have $E_g 3.55 \text{ eV}$ or absorption coefficient α =1.128x10⁴ cm⁻¹, extending far from E_g ideal for solar cell applications of 1.5 eV. E_g value is obtained from a linear extrapolation graph between the square of the absorption coefficient on photon energy.

1321 (2019) 022018 doi:10.1088/1742-6596/1321/2/022018



Figure 4 (a) Graph of absorbance of wavelengths, (b) Squared graph of absorption coefficients for energy photons for thin films of CdTe and CdTe:Cu(15%).



Figure 5 (a) Graph of transmittance to wavelength, (b) Quadratic coefficient of absorption coefficient for energy for thin films CdTe and CdTe:Cu(2%)

Transmittance graph for the wavelength of thin films CdTe and CdTe:Cu(2%), Figure 5(a), shows that both films are able to absorb light in the wavelength range of 780 nm and below. The thin film is suitable for the application of materials for solar cells that are able to absorb almost the entire visible light spectrum.

Figure 5(b) shows a graph of the square of the absorption coefficient on the energy of the thin film CdTe and CdTe:Cu(2%). From this graph, E_g CdTe thin film is 1.52 eV and E_g value of thin film CdTe:Cu(2%) is 1.48 eV or absorption coefficient $\alpha = 7.348 \times 10^4$ cm⁻¹. This value is suitable for solar cell applications [16,17].

4. Conclusion

The thin film CdTe:Cu(2%) grown by dc-magnetron sputtering method at 325 °C has better absorption performance compared to CdTe thin film grown at 325 °C/250 °C and CdTe:Cu thin film (15%) at a temperature of 250 °C. The thin film CdTe:Cu(2%) showed high absorption coefficient α =7.348x10⁴ cm⁻¹ (absorbing at a wavelength of 780 nm and below, an optical band gap of 1.48 eV). This corresponds to the morphology of flat surface grains, hexagonal crystalline structure phases and low values of microstructure parameters (degree of orientation, lattice parameters, dislocation density and micro strains). The hexagonal crystal structure phase of the CdTe:Cu(2%) thin film is suitable as a p-n junction pair with CdS which has the same stable structure phase. Heterojunction is a candidate material that can be applied to solar cells with high efficiency.

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