Structural, Chemical Composition and Optical Properties of CdTe Fabricated by Vacuum Evaporation Technique

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Abstract. CdTe polycrystalline thin films had been fabricated using vacuum evaporation technique. Their properties had been investigated using X-ray diffraction, energy dispersive spectroscopy (EDS), scanning electron microscope (SEM) and uv-vis spectroscopy. The results showed that the CdTe thin films crystalized at hexagonal structure with lattice parameters $a = 6.45$ Å and $c = 7.66$ Å. The EDS results showed that the chemical composition was non stoichiometry, slightly rich of Tellurium with Cd/Te of 0.9. It had a uniform shape with color homogenity and an optical band gap at room temperature about 1.47eV.

Introduction

Cadmium telluride (CdTe) is very important materials. It is one of the most promising photovoltaic devices applications. In general, it is a II-IV compound semiconductor which can also be applied to optoelectronic devices such as photodetectors, nuclear detectors, diode, transistor, etc. [1]. The CdTe polycrystalline films can be produced using several method such as closed space sublimation [2, 3], radio frequency (RF) sputtering [4], closed space vapor transport (CSVT) [5], molecular beam deposition [6],electrophoretic deposition (EPD) [7], and vacuum evaporation [8, 9].

The vacuum evaporation technique offers some advantages. It is a simple deposition apparatus applied under moderate vacuum conditions, it needs a high temperatures crucible but we can use a simple power supply. Previous attempts to fabricate the CdTe films by other researchers using this technique at ambient temperature resulted in a cubic structured thin films oriented to (111) plane [8, 9]. In this paper, we report our studies on the preparation of CdTe films using vacum evaporation where the films were deposited onto a glass substrate at high temperature. The films then were characterized using X-ray diffraction (XRD) to determine the crystalline structure, energy dispersive spectroscopy (EDS) to measure the chemical composition, the scanning electron microscopy (SEM) to determine the morphology of the surface, and the UV-vis spectroscopy to determine the optical characteristics such as optical band gap energy E_g.

Materials and Methods

The CdTe powder which was 250 μm and 99.99% deposition grade Sigma-Aldrich product, was put in a vacuum evaporation system and placed at a boat shape molybdenum crucible with 4.1 cm length, 1.4 cm width and 1.2 cm thickness, and heated at 1400^oC. The thin films were deposited on glass substrate heated at 370^oC. The substrate were kept at this temperatur for 2 hours under a vacuum of $3. 10^{-5}$ Torr. It was placed 10 cm above a source or a crucible for the first sample and 15 cm for the second sample.

To characterize the structure of the thin films, a Shimadzu XRD-6000 X- ray diffractometer using Cu Kα radiation with wavelength of λ = 1.54051 Å was employed. Fig. 1 shows the X-ray diffraction spectrum of CdTe with different spacer. The chemical composition of the films was determined by EDS using a JSM-6360 LA system attached to a JEOL brand scanning electron microscope. To determine the optical band gap energy,we used the transmission data of spectra made at room temperature at normal incidence in the energy range of 0.6 eV- 4.0 eV using UV

1700 Pharmaspec uv–vis spectrophotometer which was a specular reflectance attachment from Shimadzu Corporation.

Results and discussions

Structural properties and chemical composition

Fig. 1 shows the XRD spectrum of a typical CdTe. For the first sample, the patterns show a preferential orientation in the (002) direction of the hexagonal structure with $2\theta = 23.22^o$[10]. The other small peaks, $2\theta = 42.2^o$ and 45.5^o could probably associated with (103) and (200) direction respectively. For the second sample, $2\theta = 22.08^o$; 24.12^o and 39.98^o associated with (100), (002), and (110) directions. From these peaks, the lattice parameters a and c can be calculated using a relation of analytical method. This relation obtained by combining the Bragg's law and the distance between adjacent plane in the set of Miller plan indices (*hkl*) at the hexagonal structure. The lattice parameters of a hexagonal system a and c is determined by [11]

$$Sin^2(\theta) = (\lambda^2/4a^2) [(4/3)(h^2 + hk + k^2) + l^2/(c/a)^2] \tag{1}$$

These parameters a and c are constant, so Eq.(1) can be writen as

$$\sin^2\theta = A(h^2 + hk + k^2) + Cl^2 \tag{2}$$

where $A = \lambda^2/(3a^2)$ and $C = \lambda^2/(4c^2)$

The lattice parameters were calculated using the analytical method above and the results were $a = 6.50$ Å, and $c = 7.66$Å for the first sample, $a = 6.45$ Å, $c = 7.37$ Å for the second sample. These values are in a good agreement with the lattice parameter reported by others [12].

XRD spectrum shows that $2\theta = 20.9^o$ peak (marked as *) is the most probable $CdTeO_3$. In fact, in the presence of O_2 at the CdTe films growth, it generally contains a very small amount of $CdTeO_3$ [10].
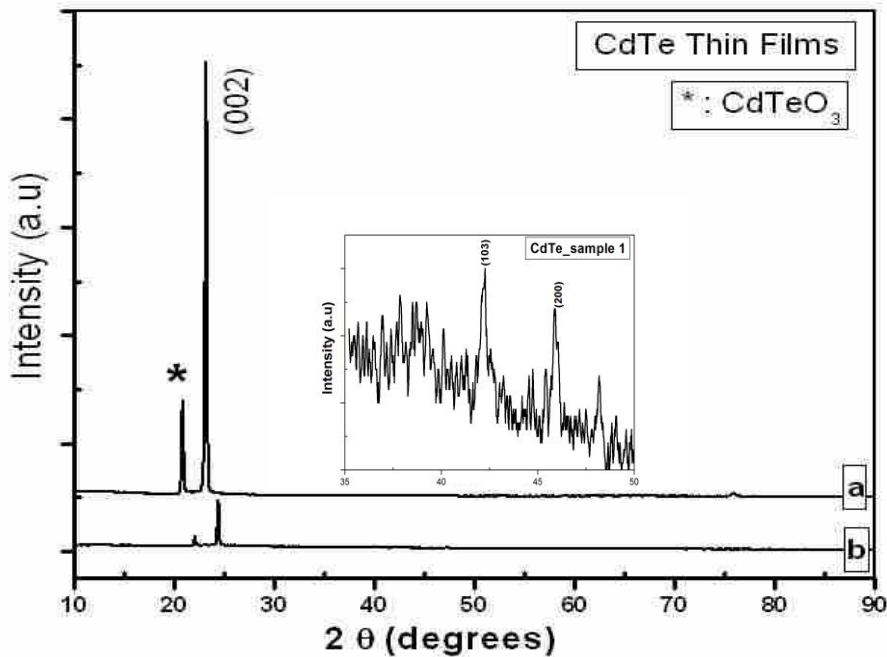

Fig.1 XRD pattern of CdTe by vacuum evaporation (a) the first sample and (b) the second sample.

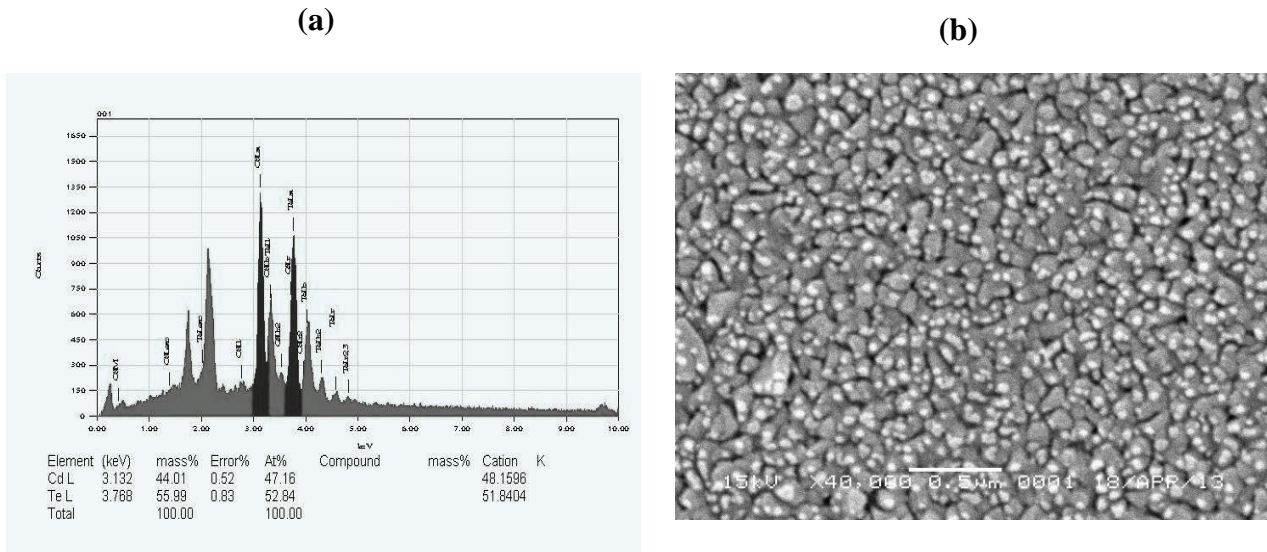| Element	(keV)	mass%	Error%	At%	Compound	mass%	Cation	K
Cd L	3.132	44.01	0.52	47.16			48.1596	
Te L	3.768	55.99	0.83	52.84			51.8404	
Total		100.00		100.00				

Fig.2 (a). Chemical composition by EDS and (b). SEM image of CdTe.

The grain size of CdTe films is also an important cell parameter. Fig. 2(b) shows the surface morphology of CdTe films prepared by vacuum evaporation technique with crucible to substrate distance of 10 cm. Its deposite consisted of grains 0.1 μm in size uniformly distributed throughout the films and it was polycrystalline in nature. Fig. 2(a) shows the results of EDS in which the element ratio of Cd and Te is 0.9.

Optical properties

Fig. 3 shows the results of the optical transmitance spectra for the first and the second samples. Transmittance (T) is the ratio of the transmission intensity (I_T) and the incidence intensity (I_o). So using Lambert's law $I_T = I_o \exp(-\alpha d)$, the absorption coefisien α can be estimated from the optical transmittance spectra using [13]

$$\alpha = (2.303/d) \log (1/T) \tag{3}$$

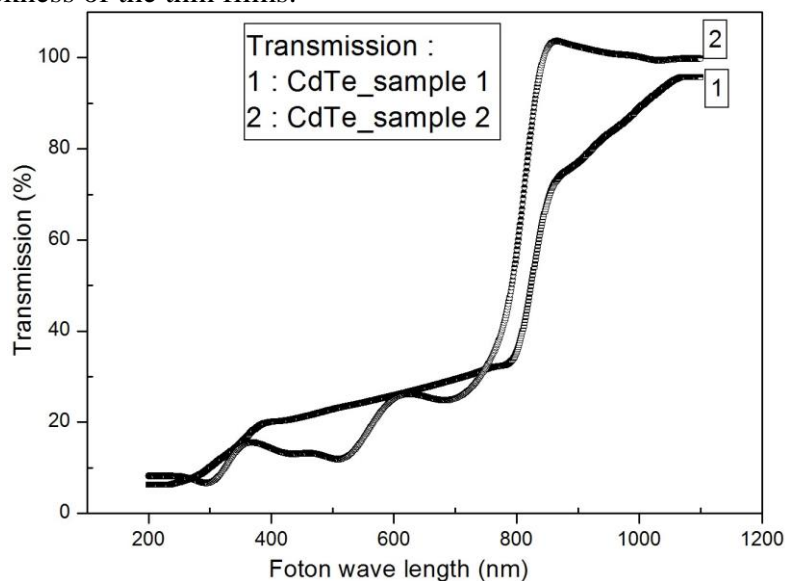Where d is the thickness of the thin films.

Fig.3 Transmission spectra of polycrystalline CdTe for the first (1) and the second (2) samples.

CdTe has a direct band gap structure, so this band gap energy E_g can be determined from the extrapolated intercept on the foton energy $h\nu$ axis using

$$(\alpha . h\nu)^2 = B^2 (h\nu - E_g) \tag{4}$$

where B is constant with a value ranging from 10^5 to 10^6 cm^{-1}eV$^{1/2}$[14]. This result is shown in Fig.4 and the band gap energy of the two samples are 1.47 eV and 1.43 eV respectively. These values agree well with the reported values in the previous studies [15].
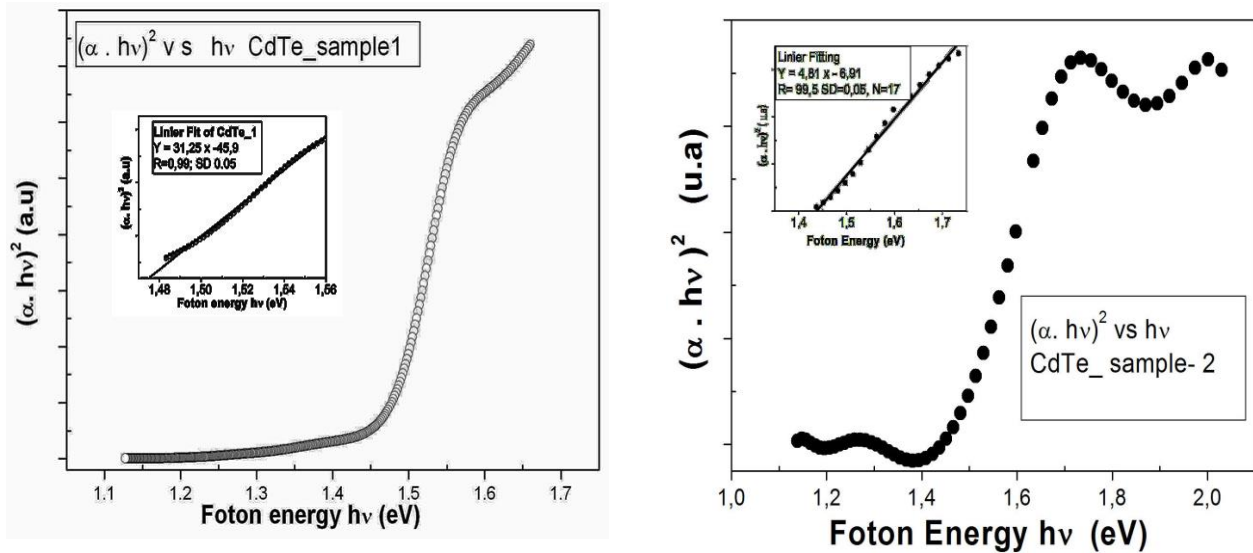

Fig. 4 Plot of $(\alpha . h\nu)^2$ versus foton energy hν for CdTe thin films.

Conclusion

CdTe polycrystalline thin films had been fabricated using vacuum evaporation technique and their properties had been characterized. The film composition was determined from a good 10 cm distance of crucible and substrate. The results of XRD showed that the CdTe had an hexagonal structure and a characteristic diffraction peak related to preferential orientation of (002). We calculated the band gap energy using the transmittance experiment data and the band gap energy of CdTe was found to be 1.47 eV.

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Advanced Materials Science and Technology

10.4028/www.scientific.net/AMR.896

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10.4028/www.scientific.net/AMR.896.497

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