Structural and optical properties of Cadmium Telluride $\text{Cd}_x\text{Te}_{1-x}$ thin film by evaporate technique

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ABSTRACT

The study reports on the structural and optical properties of II–VI group of $\text{Cd}_x\text{Te}_{1-x}$ alloying composition thin film deposited on glass substrate and prepared by evaporation technique under vacuum system of pressure $10^{-5}$ mbar. The X–ray diffraction spectrum shows that the cadmium telluride has a hexagonal polycrystalline structure with a preferential orientation along the (002) peak. The estimated grain size was around 0.16522 nm as calculated by the Scherrer equation. The energy gap values extracted from absorption spectra were around 2.4 eV. This value is larger than that for the bulk (1.44 eV) due to the inversely dependence of the energy gap on the grain size of the resulted films at the nano scale.

Keywords: $\text{Cd}_x\text{Te}_{1-x}$ alloying, thin film.

1. INTRODUCTION

$\text{CdTe}$ is a crystalline compound formed from cadmium and tellurium. It is II–VI semiconductor with zinc blende crystal structure. It is used as an infrared optical window and a solar cell material. It is usually sandwiched with cadmium sulfide to form a p–n junction photovoltaic solar cell. $\text{CdTe}$ is a direct band gap semiconductor and has a narrow band gap of 1.44 eV, which is a suitable difference of energy range for converting solar radiation into electricity. Also, this band gap can bring a large optical absorption coefficient for transporting photons. It can allow more incident light to be absorbed within a slight piece of $\text{CdTe}$. Usually, $\text{CdTe}$ shows the p–type semiconductor because the Cd vacancies are present. For the optical properties, it can emit the light with wavelength 855 nm which belongs to red color. Moreover, it has fluorescence in the visible range. $\text{CdTe}$ can be alloyed with mercury to make a versatile infrared detector material ($\text{HgCdTe}$). $\text{CdTe}$ alloyed with a small amount of zinc makes an excellent solid–state X–ray and gamma ray detector (CdZnTe). It is also applied for electro–optic modulators. It has the greatest electro–optic coefficient of the linear electro–optic effect among II–VI compound crystals. $\text{CdTe}$ doped with chlorine is used as a radiation for x–rays, gamma rays, beta particles and alpha particles. It can operate at room temperature allowing the construction of compact detectors for a wide variety of applications in nuclear spectroscopy.

The properties that make $\text{CdTe}$ superior for the realization of high performance gamma and x – ray detectors are high atomic number, large band gap and high electron mobility which result in high intrinsic (mobility – lifetime) product and therefore, high degree of charge collection and excellent spectral resolution. Bulk $\text{CdTe}$ is transparent in the infrared, close to its band gap energy (1.44 eV at 300 K) which corresponds to infrared wavelength of about 860 nm up to wavelengths greater than 20 μm, $\text{CdTe}$ is fluorescent at 790 μm. When the size of the $\text{CdTe}$ crystal is reduced to a few nanometers and below, thus making a $\text{CdTe}$ quantum dot, the fluorescence peak shifts towards through the visible range to the ultraviolet.

Usually, it is etched by many acids including hydrochloric and hydrobromic acids, forming toxic hydrogen telluride gas and toxic cadmium salts. It is a reducing agent and is unstable in air at high temperatures. It has very low solubility in water. Cadmium telluride is commercially available as a powder or as crystals. It can be made into nanocrystals.

2. Experimental work

2.1 The preparation of $\text{Cd}_x\text{Te}_{1-x}$ alloys

In the present work $\text{Cd}_x\text{Te}_{1-x}$ alloy has been synthesized using high purity elemental cadmium and tellurium is about (99.9999%) with different x content where (x=0.5 and 0.6) stoichiometric amounts of the elements are placed in a quartz ampoule. The quartz ampoule was cleaned carefully with water and alcohol respectively, to remove dust, grease, and other possible contaminants which is evacuated to a vacuum of $10^{-7}$ Torr and then sealed. The sealed ampoule is placed in a furnace and then heated at a rate of 60 °C per in steps up to 1300K. The ampoule is maintained at this temperature for about three hours and then allowed to cool slowly to room temperature. Finally the Preparation of
Cd$_x$Te$_{1-x}$ film was done by thermal evaporation. The structure of the Cd$_x$Te$_{1-x}$ alloy was examined by x-ray diffraction analysis and the composition examined by atomic absorption spectroscopy (AAS).

2.2 Measurement Instrument

Optical properties:
Absorption spectrum was measured by an Optima sp- 3000 plus UV–visible spectrophotometer with the processor Varian, Japan, this device operates within the visible and ultraviolet range of the EM spectrum thus can be used to cover the range of UV–Visible region of the EM spectrum. The absorption coefficient ($\alpha$) was calculated using Lambert law as follows:

$$\ln \frac{I_0}{I} = 2.303 \ A = \alpha d$$

where $I_0$ and $I$ are the intensities of the incident and transmitted light respectively, $A$ is the optical absorbance and $d$ is the film thickness. The absorption coefficient ($\alpha$) was found to follow the relation:

$$\alpha h\nu = A(h\nu - E_g)^n$$

where $A$ is a constant and $E_g$ is the optical energy gap. Plots of ($\alpha h\nu$)$^2$ versus the photon energy ($h\nu$) in the absorption region near the fundamental absorption edge indicate direct allowed transition in the film material. Extrapolating the straight line portion of the plot ($\alpha h\nu$)$^2$ versus ($h\nu$) for zero absorption coefficient value gives the optical band gap ($E_g$). The value of the exponent $n$ is taken as follows:
- When the absorption coefficient value is $\alpha \geq 10^4$, a direct band–band transition is obtained and the value of $n$ is taken = 2.
- While for $\alpha < 10^4$, the transition will be indirect and $n$ is taken equal to 1/2

Structure properties
CdTe crystalline structure pattern XRD was examined using SHIMADZU XRD – 6000 diffractometer. The instrument specifications are as follows:
- Target: Cu kα
- Wavelength: 1.5406 Å
- Voltage: 40 kV
- Current: 30 mA
- Range: 5 – 60 degrees
- Speed: 2 degrees/min

The interplanar distance $d$, value can be calculated in accordance to Bragg’s equation:

$$n\lambda = 2d \sin \theta$$

Where $n=1,2,3,...$ is an integer represents the order of diffraction. To calculate the particle grain size $S$, the Scherrer formula is used as follows:

$$S = \frac{k\lambda}{\beta \cos \theta}$$

Where $k$ is a constant ~0.9, $\lambda$ is the x-ray diffraction wavelength used, $\beta$ represents the full width at half maximum (FWHM) and $\theta$ is the diffraction angle.

Thickness measurement
Interferometer was used to measure the thickness of CdTe thin films. Using a He–Ne laser (wavelength of 632.8 nm), the film thickness, $t$, can be determined by the following formula:

$$t = \frac{b\lambda}{a}$$

Where ($a$) represents the fringe width, ($b$) is the fringe spacing, and $\lambda$ is the wavelength of the laser light used.
3. Result and discussion

The x-ray diffraction spectrum for cadmium telluride, shown in figure 1, was obtained in the 2θ range of 10° – 60° (0.05 degree step with 5 deg./min. speed) using CuKα target, and radiation of 1.5406 Å wavelength. The spectrum data shows that the cadmium telluride has a hexagonal polycrystalline structure with a preferential orientation along the (002) peak. The Table 1 gives the 3 dominant strongest peaks with their d spacing, FWHM and diffraction angle values. The grain size, S=0.16522 nm, was evaluated using Scherrer’s equation for the (002) peak. UV_VIS absorption spectrum of Cd_{x}Te_{1-x} where x= 0.5 and 0.6 are shown in figure 2 and figure 3 respectively. The spectrum shows that the sample is highly absorbed in UV region around 350 nm whereas it still absorbed in the visible region up to 500 nm and it becomes transparent beyond this wavelength. It can be noticed from figure that the spectrum will be shifted to UV region with increase the concentration of Cd. The absorption spectrum is normally used to evaluate the energy gap \(E_g\) of the sample under study following the calculation of the absorption coefficient. Figure 4 shows the relationship of \((\alpha h\nu)^2\) versus the photon energy \((h\nu)\) where the resulted energy gap values were around 2.4 eV. For x=0.5 and 3.2 eV for x=0.6.

4. Conclusions:

Cadmium telluride is a promising II–VI semiconductor material in view of its unique properties which made it a real candidate for many applications. The crystalline structure of the current CdTe thin films is hexagonal polycrystalline structure with (002) peak of dominant intensity. The obtained films are of crystal structure in agreement with JCPDS standards (CAS number: 1306-25-8). The energy band gap measurements showed the effect of reduced grain size on the \(E_g\) value which were around 2.5 eV.

![XRD spectrum of cadmium telluride](image)

**Figure 1: XRD spectrum of cadmium telluride**

**Table 1:** shown all peaks and its Bragg's angle, interplanar distance, and full width half at maximum.

<table>
<thead>
<tr>
<th>No.</th>
<th>Peak no.</th>
<th>2Theta (deg.)</th>
<th>d (Å)</th>
<th>FWHM (deg.)</th>
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<td>3.39240</td>
<td>0.50000</td>
</tr>
</tbody>
</table>
Figure 2: Shows the absorbance (top) and transmittance (bottom) spectra for Cd$_x$Te$_{1-x}$ where $x=0.5,0.6$. 
Figure 3: Absorption coefficient variation with the photon energy for x=0.5 (top) and x=0.6 (bottom)

References:
[1.] http://wikipedia.com/cadmium_telluride

AUTHOR
Dr. Mohammed T. Hussein completed his Ph.D. at the physics department in laser spectroscopy from Complutense University – Madrid-Spain in 1995. His research interests lie in the field of organic semiconductor and molecular spectroscopy. He is currently a member of the Nanotechnology & Optoelectronics Research Group at the Physics department of Baghdad University.