Doping Ratio Of Silver Dependent On The Structure And Optical Properties Of Thin Cadmium Telluride Films

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Abstract—In this work, we are studying the effect of doping ratio on the structure and the optical properties of CdTe: Ag thin films which were prepared by thermal evaporation technique in vacuum with rate deposition (3.42 Å/sec) and thickness (≈300 nm), we studying the influence of doping by Silver with different ratios (1%, 2%, 3%) at substrate temperature (300K) on the structural and optical properties of Cadmium Telluride thin films. The structural properties of the films have been studied by using X-ray diffraction. The optical measurements indicated that CdTe: Ag films have direct optical energy gap (E_g), and it decreases from 1.55eV to 1.51eV with the increase of doping ratio (Undoped – 3%). The optical constants refractive index (n), extinction coefficient (k), absorption coefficient (α) and dielectric constants (ε_r and ε_i) were also studied.

Keywords—CdTe: Ag , energy gap, XRD, Thermal evaporation.

Introduction

Cadmium Telluride (CdTe) is an important compound semiconductor of II-VI group. It is a potential candidate for having suitable applications in the areas of polycrystalline thin films, IR detector, photovoltaic and optoelectronic applications [1]. Thin films of III-V semiconductors like GaAs, InP, and GaN, as well as II-VI semiconductors like CdTe, ZnTe, and ZnO exhibit high efficiencies, they have high absorption coefficient and have direct band gap, the values of which correspond to the wide range of solar spectrum [2]. Cadmium Telluride (having band gap energy of 1.5 eV at room temperature) is a direct band gap material. The very high absorption coefficient of CdTe (more than 10^5 (cm^-1)) at a wavelength of 700 nm makes even a two micron thick layer absorb more than 90% of light energy corresponding to the band gap energy of CdTe [3] thus making it useful for solar cell applications. Polycrystalline CdTe absorber layers may be deposited on CdS window layers by a variety of techniques [4-8] CdTe thin film with the appropriate metal atoms such as In, Zn, Ag, Bi, Sb, Al, etc., produces considerable changes in their structural and physical properties that make it very good candidate material in the technology of thin film devices (9).

Experimental Work:

The films of Cadmium Telluride doped with Silver were prepared by thermal evaporation technique using coating unit in a vacuum about 2×10^-5 Torr. A specific weight from Cadmium Telluride powder (99.9% pure) must be taken and put it in a special evaporation molybdenum boat, after evaporation Cadmium Telluride thin films we take different ratio (1%) , (2%) , (3%) from this weight from Silver and put it in other molybdenum boat. We used thermal diffusion method to doped Cadmium Telluride thin films with Silver, the rate of evaporation was ≈ 3.42 Å/sec and the film thickness in the range of (300) nm was measured by interference method and the substrate glass was placed directly above the source at a distance of nearly 18 cm after cleaned the glass.

The optical band gap Eg can be estimated from the following relation known as the Tauc relation [10]:

\[ \alpha h\nu = B( h\nu - E_g)^n. \]  

(1)

Where B is a constant, ν is the transition frequency and the exponent n characterizes the nature of band transition. n= 1/2 and 3/2 corresponds to direct allowed and direct forbidden transitions and n = 2 and 3 corresponds to indirect allowed and indirect forbidden transitions, respectively. For all the films the best straight line is obtained for n equal to ½, which is expected for direct allowed transition.

The optical constant absorption coefficient (α), refractive index (n), extinction coefficient (k) and real (ε_r) and imaginary part (ε_i) of dielectric constant can be calculated from the following equation [11].

\[ \alpha = 2.303 \frac{A}{t}. \]  

(2)

Where (t) is the film thickness and (A) is the optical absorbance.

The extinction coefficient (k) can be determined by using the equation [12]:

\[ k = \frac{\alpha \lambda}{4\pi}. \]  

(3)

Where (λ) is the wavelength of the incident radiation.
The dielectric constant real part ($\varepsilon_r$) and imaginary part ($\varepsilon_i$) can be calculated by using equation [13]:

$$\varepsilon_r = n^2 - k^2. \quad (4)$$

$$\varepsilon_i = 2nk. \quad (5)$$

Where ($n$) is the refractive index was obtained from the following relation [14].

$$n = \left[ \frac{4R}{(R - 1)^2 - k^2} \right]^{\frac{1}{2}} \left( \frac{R + 1}{R - 1} \right). \quad (6)$$

Where ($R$) is the reflection.

**Result and Discussion:**

Figure (1) and table (1) show the XRD spectra obtained at different doping ratio for CdTe:Ag films. The XRD pattern for Cadmium Telluride doped with Silver films at different doping ratio (Undoped, 1%, 2% and 3%) shows a polycrystalline structure of all samples before and after doping. The peaks represent is cubic structure having a zinc blend type with atomic prevalent growth direction peak at [111]. This figure indicates According to the American standard for testing materials (ASTM) cards. In general we notice decreases in value of intensity peak at [220], [311], while at [111] we find increases in value of intensity peak for the samples before and after doping. This may be due to improving the crystallite structure after increases the doping ratio of Silver, also we can see the value of ($2\theta$) after doping with different ratio of Silver toward to higher value due Silver atoms occupy sites within the crystal structure which that lead to a change in values of ($d_{hkl}$) Which causes a shift of ($2\theta$) values. This result agrees approximately with the result reported by [15,16].
Table 1: X-ray diffraction data for CdTe films with different doping ratio by Silver.

<table>
<thead>
<tr>
<th>Sample</th>
<th>(hkl)</th>
<th>2θ° Observed</th>
<th>d(A°) Observed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Undoped</td>
<td>111</td>
<td>23.750</td>
<td>3.737</td>
</tr>
<tr>
<td></td>
<td>220</td>
<td>39.320</td>
<td>2.285</td>
</tr>
<tr>
<td></td>
<td>311</td>
<td>46.426</td>
<td>1.956</td>
</tr>
<tr>
<td>1%</td>
<td>111</td>
<td>23.742</td>
<td>3.739</td>
</tr>
<tr>
<td></td>
<td>220</td>
<td>39.168</td>
<td>2.289</td>
</tr>
<tr>
<td></td>
<td>311</td>
<td>46.386</td>
<td>1.951</td>
</tr>
<tr>
<td>2%</td>
<td>111</td>
<td>23.760</td>
<td>3.744</td>
</tr>
<tr>
<td></td>
<td>220</td>
<td>39.342</td>
<td>2.286</td>
</tr>
<tr>
<td></td>
<td>311</td>
<td>46.468</td>
<td>1.949</td>
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<tr>
<td>3%</td>
<td>111</td>
<td>23.768</td>
<td>3.742</td>
</tr>
<tr>
<td></td>
<td>220</td>
<td>39.380</td>
<td>2.294</td>
</tr>
</tbody>
</table>

The optical energy gap values (Eg) for CdTe:Ag films have been determined. A plot of (αhν)² versus photon energy for CdTe:Ag films at different doping ratios (undoped, 1%, 2%, 3%) are shown in Fig.(2) and table(2). The plot is linear indicating a direct band gap nature of the film. Extrapolation of the line to the photon energy axis gives the band gap. The values of the optical energy gap for CdTe:Ag films are decrease from (1.55 eV) to (1.51 eV) when increase the doping ratios from (undoped to 3%). This is due to the increase of the density of localized states in the Eg, which causes a shift to lower values. This result agrees approximately with the result reported by [17,18].

Figure 2: Variation of energy gap for CdTe:Ag films as a function of different doping ratio with Silver

The Figure (3) refer to transmission of CdTe:Ag films in the range between (300-1000) nm. The transmittance spectra show a decrease when increases the doping ratio of Silver because of the effect of impurities atoms, which is working on the composition of localized levels in the energy gap.

Figure 3: The optical transmission for CdTe:Ag films as a function of wavelength at different doping ratio with Silver

From Figure (4) we can see the beaver reflectance spectrum of Cadmium Telluride films doped with different ratio of Silver as a function of wavelength. From this figure we can observed increasing by reflectance with increases the wavelength for short wavelength but at long wavelength we can see decreasing reflectance with increases the wavelength. This result similar with the result reported by [18].

Figure 4: The reflectance spectrum for CdTe:Ag films as a function of wavelength at different doping ratio with Silver

The absorbance spectrum for CdTe:Ag films shows in figures (5). The absorbance spectrum shifts to longer wavelengths with increasing of doping ratio for all the samples and the absorbance increases with increasing of doping ratio and this may be due to improving the crystallite size and decreasing the transmittance, which agree with result obtained by [18].

Figure 5: The absorbance spectrum for CdTe:Ag films as a function of wavelength at different doping ratio with Silver
Figure 5. The absorbance spectrum for CdTe:Ag films as a function of wavelength at different doping ratio with Silver

We can notice that the absorption coefficient ($\alpha$) for CdTe:Ag films in general increases with increasing of doping ratio. This behavior is show in figures (6).

Figure 6. Absorbance coefficient for CdTe:Ag films as a function of wavelength at different doping ratio with Silver

Figure (7) show the variations in refractive index ($n$) as a function of wavelength for CdTe:Ag. The refractive index increases with increases the doping ratio at longer wavelength because increase the level energies in forbidden gap.

Figure 7. Refractive index for CdTe:Ag films as a function of wavelength at different doping ratio with Silver

The extinction coefficient ($k$) increases with the increase of doping ratio for Cadmium Telluride doped with Silver films as shown in Fig.(8) and this may be due to increasing the absorption coefficient which shown in Fig.(6).

Figure 8. Extinction coefficient for CdTe:Ag films as a function of wavelength at different doping ratio with Silver

The dielectric constant real part ($\varepsilon_r$) and imaginary part ($\varepsilon_i$) with the increases doping ratio for the films are shown in Fig. (9) and in Fig.(10)corresponds. The real part($\varepsilon_r$) increases with the increase of doping ratio, and this attributed to the same reason mentioned previously for the refractive index, also imaginary part ($\varepsilon_i$) increases with the increase of doping ratio and this is due to the similar interpretation discussed previously for the extinction coefficient. This result for all optical constant ($\alpha$, $n$, $k$, $\varepsilon_r$, $\varepsilon_i$) agree with result obtained by [18].

Figure 9. Dielectric constant real part for CdTe:Ag films as a function of wavelength at different doping ratio with Silver
Figure 10. Dielectric constant imaginary part for CdTe:Ag films as a function of wavelength at different doping ratio with Silver

Table 2: The optical properties parameters of MnS:Al thin films at different annealing temperatures when λ=700 nm.

<table>
<thead>
<tr>
<th>Sample</th>
<th>$E_g$ (eV)</th>
<th>$\alpha$ x10$^4$(cm$^{-1}$)</th>
<th>n</th>
<th>k</th>
<th>$\varepsilon_r$</th>
<th>$\varepsilon_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Undoped</td>
<td>1.55</td>
<td>5.8</td>
<td>8.99</td>
<td>0.32</td>
<td>80.8</td>
<td>5.8</td>
</tr>
<tr>
<td>1%Ag</td>
<td>1.53</td>
<td>6.4</td>
<td>928</td>
<td>0.35</td>
<td>86.1</td>
<td>6.6</td>
</tr>
<tr>
<td>2%Ag</td>
<td>1.52</td>
<td>6.8</td>
<td>9.42</td>
<td>0.38</td>
<td>88.6</td>
<td>7.2</td>
</tr>
<tr>
<td>3%Ag</td>
<td>1.51</td>
<td>7.3</td>
<td>9.47</td>
<td>0.41</td>
<td>89.5</td>
<td>7.7</td>
</tr>
</tbody>
</table>

Conclusion:
The effect of change doping ratio on the structure and optical properties of CdTe:Ag thin films deposited by thermal evaporation technique were studied. The structure of all films at different doping ratio is cubic, the films show a direct optical energy gap ($E_{opt}^{g}$), and it decreases with the increase of doping ratio. All films exhibit high transmittance. The transmittance spectra and show a decrease when the doping ratio increases, while absorbance spectrum, the absorption coefficient, the refractive index, the extinction coefficient, dielectric constant real part ($\varepsilon_r$) and imaginary part ($\varepsilon_i$) increase with the increase of doping ratio. so we can used CdTe:Ag films as solar cell or IR window.

References