The Optical and Surface Morphology Properties of AgInTe$_2$

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ABSTRACT

AgInTe$_2$ (AIT) thin films prepared by using vacuum thermal evaporation technique, of thickness 150 nm, with deposition rate 1.8±0.2 nm/sec on glass of substrate with pressure ($10^{-5}$) mbar and at room temperature. In the range 473-673 K all samples has been heat treatment. The AIT properties of optical thin films would been studied like (coefficient of absorption, index of refractive, coefficient of extinction, real and imaginary dielectric constant) by using Measurement spectra of absorption and transmission. Results of the optical constants showed that it is wide applications as an photovoltaic applications and optoelectronic devices.

Keywords: AgInTe$_2$ thin films, Thermal evaporation, Optical properties, transmission

1. INTRODUCTION

The semiconductors ternary (ABX$_2$) show a much richer of chemical and physical properties [1]. The ternary (ABX$_2$) semiconductors have wide optical band gaps range and motilities of carrier, has led to their appearance importance device materials, including solar cells of photovoltaic light-emitting diodes [1,2], and in several nonlinear optical devices [3,4].
The AgInTe$_2$ thin films which was prepared on glass substrates prepared by using thermal vacuum evaporation at room temperature. On annealing at 473 and 573 K.

The thin films optical properties transmittance and reflectance at normal incidence in the wavelength range 100–1100 nm were investigated by using spectrophotometric measurements. The AgInTe$_2$ index of refractive (n) and the index of absorption (k) were specified from the absolute values of the measured transmittance and reflectance. It was found (n) and (k) showed that they rely depend significantly on the heat treatment temperature.

2. EXPERIMENTAL DETAILS

The AgInTe$_2$ films have been deposited on glass substrate by thermal vacuum evaporation using Edwards – Unit 306 system at room temperature with 4.5×10$^{-5}$ mbar. The films thickness were specified with Precisa-Swiss microbalance using a weighing method and it found to be about 150±10 nm, with rate of deposition about 1±0.1 nmsec$^{-1}$. The distance between the substrate and the boat is 18 cm. Atomic force microscopy (AFM) measurements were performed using SPM-AAA3000 contact mode spectrometer, Angstrom from the Advanced Inc. Company, USA, to determine the grain size and nanocrystal line topography of the films. Optical transmission measurements were made with (UV/Visible 1800 spectrophotometer).

By using Scherrer's formula were calculated Crystallite size (D) of the as-deposited and annealed films [5]:

$$D = \frac{0.9\lambda}{\beta \cos \theta} \quad \text{.......................... (1)}$$

where: (λ = 1.54059 Å) wavelength used in the X-Ray, $\beta_r$ (WFHM) is the full width at half maximum of diffraction peak measured in radians units, $\theta$ is the diffraction angle (Bragg angle).

The density of dislocation ($\delta$) is defined as the lines dislocation length per unit crystal volume and has been calculated using the equation [6]:

$$\delta = \frac{1}{D^2} \quad \text{..................(2)}$$

where: the $\delta$-value is crystallization level criterion

The crystallites number of per unit surface area ($N_o$) of the film was determined using the equation [6]:

$$N_o = \frac{t}{D^3} \quad \text{.......................... (3)}$$

where: the t is the films thickness.

The coefficient of absorption ($\alpha$) of a thickness film (t = 150 nm) can be calculated from the transmittance spectrum using the following equation [5]:

$$\alpha = 2.303 \frac{A}{t} \quad \text{.......................... (4)}$$
where: \( t \) is the thickness of film and \( A \) is the absorbance, which is calculated from the relation [5]:

\[
A = \log(1/T)
\]

(5)

where: \( (T) \) is the transparence.

The absorption fundamental, which agrees almost exactly to excitation an electron from the valence band to the conduction band and can be used to specify the nature and value of the optical band gap and could be calculating for using the equation [6]:

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

(6)

where: \( B \) is constant depending on the semiconductor type, \( \alpha \) [cm\(^{-1}\)] is the coefficient of absorption, \( h\nu \) is the photon energy and \( E_g \) [eV] is the optical band gap. The \( n \) parameter is index depend to the material nature and specified by the optical transition contain in the process of absorption, it determined the allowed direct \((n = 1/2)\) [7].

When electromagnetic radiation falls on a surface, part of it is reflected, and part of it is absorbed and transmitted [8]. Optical constants are important characteristics of the material as they describe their optical behavior so vaporized films have optical properties and are based on evaporation technology [11]. The optical constants of the material are the index of refractive \((n)\), the coefficient of extinction \((k)\), real \((\varepsilon_1)\) and imaginary parts \((\varepsilon_2)\) of dielectric constant. The index of refractive \((n)\) can be calculated by using the equation [9]:

\[
 n_o = \left[ \left( \frac{1+R}{1-R} \right)^2 - (k_o^2 + 1) \right]^{1/2} + \frac{1+R}{1-R}
\]

(7)

where: \( R \): is the reflectance and given by the equation [10]:

\[
R = 1 - (A + T)
\]

(8)

Refractive index is an important factor in the research of the optical properties of materials, Because it is an important factor in optical communication and in the design of spectroscopic devices [11].

The Extinction coefficient \( k \) is the exponential decay of electromagnetic radiation intensity which represents the amount of energy absorbed in the thin film and can be determined by using the equation [12]:

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

(9)

where: \( \lambda - \) is the incident radiation wavelength.

Complex electronic dielectric constant \((\varepsilon)\) describes the fundamental electron excitation spectrum of the films was by means of a frequency dependent of it, and it is defined as [13]:

\[
\varepsilon = \varepsilon_1 - i \varepsilon_2
\]

(10)
Both the real and imaginary parts of the dielectric ($\varepsilon_1$ and $\varepsilon_2$) constant are related to the values of $n$ and $k$, and can be calculated by using the equations [13]:

$$\varepsilon_1 = n^2 - k^2 \quad \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots (11)$$

$$\varepsilon_2 = 2nk \quad \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots (12)$$

3. RESULTS AND DISCUSSION

Figure (1) showed the XRD patterns for samples with thicknesses 150 nm and annealed at 473-673 K. The films appear to have been characterized by three major crystal peaks, the first peak appeared at $2\theta = 23.976^\circ$, second peak appeared at $2\theta = 39.7913^\circ$. On comparison with ICDD (card no. 00-023-0638). The first peak was specified 112 be the property of structure AgInTe$_2$ with the identified orientation and the second peak 220 orientation specified, and that main all films have poly crystalline structure.

![Figure 1. XRD patterns of (a) RT, Ta (473K, 573K, 673K).](image)

The lattice constant calculated for the peaks of 112 and 220 of AgInTe$_2$ averaged to $a = 6.59 \text{ Å}$, $b = 12.61 \text{ Å}$. From the figures it is clear that there is no variance in position of peak otherwise, the temperature annealing 673 K have maximum intensity, that mean the crystallinity of the films is increased with increasing the temperature. Table 1 showed that the grain size of AgInTe$_2$ films increases when temperature increasing. The $\delta$-value is crystallization level criterion from Table 1. Lower $\delta$-values point out the films have higher crystallinity levels, so $\delta$ is the measure of the quantity of defects crystal and the value of
Dislocation density gated in this work is found to be equal to $6.22 \times 10^{14}$ lines/m$^2$ for films. In the present work confirms obtained small value of $\delta$ that mean a good crystallinity of the fabricated AgInTe$_2$ film by this method.
Figure 2. AFM-3D images of (a) R.T, Ta (b) 473K, (c) 573K, (d) 673K.
To study the change in the surface morphology of the films we use Atomic force microscopy (AFM) scans. AFM images are shown in Fig. 2 and these images show that the film is homogeneous, with no holes and notes in all the films. We can observe the surface roughness of the films is changed with the increase of temp and that indicate the increase in surface roughness affects the structural properties of the surface of the films as well as changes in the electronic and optical transformations of the material [14]. Table 2 shown the grain size and the root-mean-square (RMS) roughness of the samples.

Optical transmittance spectra with a wavelength of 400 nm to 1100 nm are shown as in Fig. 3 of the AgInTe$_2$ thin films at room temperature and annealed. As the temperature increases, optical transmittance decreases. In usually the transmittance of optical increases with increased the wavelength, so increase of temperature annealing lead to shifting in the wavelength for the region where that the transmittance increases. We see that is the transmittance is becoming very high for all the range of annealing temperature at the wavelength longer than 800 nm.

![Figure 3. Transmittance spectra of AgInTe$_2$](image)

Absorption spectra of AgInTe$_2$ thin films at room temperature and annealed shown in Fig. 4. The absorption spectra of thin film depend mainly on surface roughness and temperature [15]. As seen in Fig. 4, that the high absorption peaks shifts to the lower wavelength when Increase temperature annealing the absorption value increase and it changes with a range of temperature because heat treatment leads to rearrangement the atoms in the structure [16].

Fig. 5. are shown the reflectance spectra of AgInTe$_2$ thin films at room temperature and annealed temperature. Showed that the average reflection of the AgInTe$_2$ film increased rapidly in the visible area of the film 400-800 nm while decreasing with the wavelength increase of the range 800-900 nm as the temperature increased.
Figure 4. Absorption spectra of AgInTe$_2$ thin films at different annealing temperature.

Figure 5. Reflectance spectra of AgInTe$_2$ thin films at different annealing temperature.

The change in film reflection indicates that the refractive index of AgInTe$_2$ films changes with temperature. The AgInTe$_2$ refractive index of the film in the range of 370-675
nm showed the lowest value at room temperature in the visible range, but at 473 K the films showed the highest value in the NIR.

Absorption coefficient is measured the material ability to absorb light and it is a very important function of the band gap energy and photon energy [17].

Fig. 6 are shown the optical absorption coefficient variation with photon energy for different temperature.

![Figure 6. Variation of absorption coefficient as a function of photon energy](image)

By using equation (4) we calculated the values of absorption coefficient in the order of $10^4$ cm$^{-1}$. The $\alpha$ absorption coefficient decreases $\alpha$ with increasing wavelength and the absorption coefficient ($\alpha$) show high value that mean there is a high probability of the allowed direct transition, and ($\alpha$) decreases with increase of wavelength.

Fig. 7 are shown the optical band gap energy $E_g$ and it has been found that the temperature affects in the energy band gap $E_g$. The direct band gap at RT is 1.5 eV and this value is consistent with many reports. Band gap values were found to decrease with increasing temperature because increasing the width of localized state in the optical band gap. Also, it is shown in Table 3. And we found that the annealing temperature of the AIT affects the band gap energy ($E_g$). This can be explained by the rearrangement of atoms in the structure and annealing of some defects. These defects appear as deep and shallow level in the band gap of the elaborated semiconductors material [18].

Figure 8 showed the variation of refractive index with photon energy were calculated using Eq. (7) when increasing of photon energy (decreases in wavelength) the refractive index increases that indicating that all the films are showing a normal dispersion behavior in the range 1.1-2 eV corresponding to the wavelength in the range 620-950 nm. From Table 3 we show that the refractive index decrease with annealing films.
Fig. 9 shows the extinction coefficient \((k)\) variation of as a function of photon energy. By increasing the photon energy the absorption coefficient will increase and increasing the extinction coefficient from Table 3 showed that. So, The behavior of \((k)\) is matching almost to the corresponding absorption coefficient \((\alpha)\) because of the extinction coefficient mainly depends on \((\alpha)\) from the Eq (9).
Figure 9. Extinction coefficient variation as a function of photon energy.

Fig. 10 are showed the real dielectric constant ($\varepsilon_1$) has a behavior roughly similar to the corresponding refractive index (n) because of the small value of ($k^2$) and that is clear from Eq. (11). Curves increase to the maximum peak and then begin to decrease as photon energy increases for all the films. Also, the peaks of $\varepsilon_1$ where shift to the lower photon energy with the increase the temperature.

Figure 10. Real part of dielectric constant as a function of photon energy.
Fig. 11 are showed the real dielectric constant ($\varepsilon_2$) has a behavior roughly similar to the corresponding extinction coefficient because of $\varepsilon_2$ depends on the extinction coefficient and that is clear in Eq. (12). Also, the peaks of $\varepsilon_2$ where shift to the lower photon energy with the increase the temperature.

![Graph](image)

**Figure 11.** Imaginary part of dielectric constant as a function of photon energy

The change ($\varepsilon_1$) with photon energy refer to some interactions between the photons and the electrons in the prepared films and ($\varepsilon_2$) related to the density of states within the forbidden gap of semiconductor materials and Table 3 are shown the values of the dielectric constant.

**Table 1.** XRD, results of AIT thin films for the 112 preferred orientation peak.

<table>
<thead>
<tr>
<th>Thickness (nm)</th>
<th>$\theta$ (112)</th>
<th>$a$ (Å) observed</th>
<th>$c$ (Å) observed</th>
<th>FWHD (112)(deg.)</th>
<th>D (nm)</th>
<th>$N_0*10^{12}$ (m$^{-3}$)</th>
<th>$\delta*10^{14}$ (m$^{-2}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>RT</td>
<td>23.90</td>
<td>6.85</td>
<td>12.52</td>
<td>0.281</td>
<td>28.88</td>
<td>11.98</td>
<td>6.22</td>
</tr>
<tr>
<td>Ta 473K</td>
<td>23.93</td>
<td>6.82</td>
<td>12.56</td>
<td>0.276</td>
<td>29.41</td>
<td>11.56</td>
<td>5.89</td>
</tr>
<tr>
<td>Ta 573K</td>
<td>23.95</td>
<td>6.89</td>
<td>12.59</td>
<td>0.253</td>
<td>32.08</td>
<td>9.71</td>
<td>4.54</td>
</tr>
<tr>
<td>Ta 673K</td>
<td>23.96</td>
<td>6.93</td>
<td>12.62</td>
<td>0.231</td>
<td>35.14</td>
<td>8.09</td>
<td>3.45</td>
</tr>
</tbody>
</table>
Table 2. AFM analysis, the crystal grain size, surface roughness of AgInTe$_2$

<table>
<thead>
<tr>
<th>Thin films</th>
<th>Grain size, D (nm)</th>
<th>(RMS) roughness (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>RT</td>
<td>195</td>
<td>8.0569</td>
</tr>
<tr>
<td>Ta 473K</td>
<td>197</td>
<td>13.688</td>
</tr>
<tr>
<td>Ta 573K</td>
<td>210</td>
<td>16.964</td>
</tr>
<tr>
<td>Ta 673K</td>
<td>229</td>
<td>21.061</td>
</tr>
</tbody>
</table>

Table 3. Energy gap, coefficient of extinction, index of refractive and $\varepsilon_1$, $\varepsilon_2$ AgInTe$_2$.

<table>
<thead>
<tr>
<th></th>
<th>Eg (eV)</th>
<th>$\lambda$ (nm)</th>
<th>$k$</th>
<th>n</th>
<th>$\varepsilon_1$</th>
<th>$\varepsilon_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>RT</td>
<td>1.5</td>
<td>825</td>
<td>0.3781</td>
<td>7</td>
<td>48.87</td>
<td>5.29</td>
</tr>
<tr>
<td>Ta 473K</td>
<td>1.43</td>
<td>865</td>
<td>0.459</td>
<td>8.746</td>
<td>76.28</td>
<td>8.045</td>
</tr>
<tr>
<td>Ta 573K</td>
<td>1.34</td>
<td>925</td>
<td>0.627</td>
<td>8.27</td>
<td>68.04</td>
<td>11.136</td>
</tr>
<tr>
<td>Ta 673K</td>
<td>1.28</td>
<td>965</td>
<td>0.867</td>
<td>7.123</td>
<td>50</td>
<td>12.35</td>
</tr>
</tbody>
</table>

4. CONCLUSIONS

The AgInTe$_2$ were deposited by thermal vacuum evaporation. The structure of AgInTe$_2$ thin films was poly crystalline and grain size increased with increasing the temperature. The change in temperature has affected topography and optical properties. The highest absorption value was found in the visible region. From the transmission spectra, the absorption coefficient was calculated within the wavelength of 400 to 1100 nm. In the higher energy region Absorption coefficient was obtained and the absorption rate is max close the absorption edge of the order of $10^5$ cm$^{-1}$. The values of optical band gap were found to be decrease from 1.5eV to 1.28eV with increase the temperature. In this work has been investigated the optical constants of the films depend on the temperature. Finally, the AgInTe$_2$ films was suitable application in various optoelectronic devices as photodetector and photocell.

References